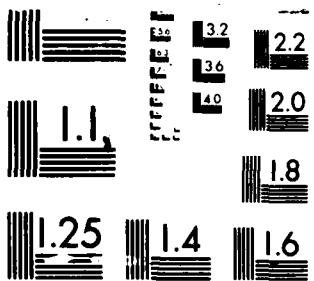


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**A FAMILY OF ALGORITHMS FOR THE
ESTIMATION OF THE PARAMETERS OF THE STABLE LAWS AND
THE PARAMETERS OF ATTRACTING STABLE LAWS**

by

**T. A. Delehanty
and
A. S. Paulson**



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DESCRIPTION AND PURPOSE

Potential application of the stable laws has long been hindered by the unavailability of generally available, well-documented algorithms. This paper removes this deficiency by presenting an algorithm for estimation of stable law parameters, with the goal of facilitating the application of stable laws in modeling and inference frameworks. The stable laws have steadily increased in importance to the statistical community since the paper of Mandelbrot (1963). Their role as the only laws possessing domains of attraction makes the stable laws an appealing probabilistic model, and they are capable of modeling a wide range of skewness, heavy tailedness, and central peakedness. Procedures for estimation of stable law parameters have been described by Mandelbrot (1963), DuMouchel (1971), Fama and Roll (1971), Paulson, Holcomb, and Leitch (1975), Koutrouvelis (1980,1981), Feuerverger and McDunnough (1981a,1981b), and Brockwell and Brown (1981). Because of the intractability of stable densities, attention has centered in recent years on Fourier-based procedures, using the empirical characteristic function. Such procedures should have an adaptive nature (Paulson, Holcomb, and Leitch, 1975; Paulson, Delehanty, and Brothers, 1982; Paulson and Delehanty, 1982).

We present an iterative and adaptive algorithm for joint estimation of stable law parameters, using the empirical characteristic function. The algorithm is flexible in that either of two procedures may be selected, and subsets of the parameters may be allowed to vary freely, with others constrained or held constant. The statistical rationale for the procedures is described in the companion paper by Paulson and Delehanty (1982). The algorithm may also be used to provide informal estimates of the parameters.

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estimation

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of the stable law to which a sample distribution is attracted.

THEORY AND NOTATION

Nondegenerate stable random variables X may be defined by the characteristic function

$$\phi(u) = E(\exp(iuX)) = \exp\{iu\mu - |\sigma u|^\alpha(1 + i\beta \operatorname{sgn}(u) \chi(u, \alpha))\}, \quad (1)$$

where $i^2 = -1$, $0 < \alpha \leq 2$, $|\beta| \leq 1$, $\sigma > 0$, and

$$\chi(u, \alpha) = \begin{cases} \tan \frac{\pi\alpha}{2}, & \alpha \neq 1 \\ \frac{2}{\pi} \log|u|, & \alpha = 1. \end{cases} \quad (2)$$

Here α , the characteristic exponent, is a measure of heavy tailedness and central peakedness, β is a skewness measure, σ is a scale parameter, and μ is a location parameter unless ($\alpha=1$, $\beta \neq 0$), when the function of location parameter is assumed by $\mu + \frac{2}{\pi} \beta \log \sigma$. The only stable laws whose densities are expressible in closed form are the Gaussian ($\alpha=2$, $\beta=0$), the Cauchy ($\alpha=1, \beta=0$), and the reciprocal of a χ^2 variate on one degree of freedom ($\alpha=\frac{1}{2}, \beta=-1$).

Let X_1, \dots, X_n be a stable random sample. The empirical characteristic function is

$$\phi_n(u) = n^{-1} \sum_{j=1}^n \exp(iuX_j). \quad (3)$$

Let $\psi(u) = \operatorname{Re} \phi(u) + \operatorname{Im} \phi(u)$, $\psi_n(u) = \operatorname{Re} \phi_n(u) + \operatorname{Im} \phi_n(u)$. Estimators interior to the parameter space can be viewed as zeros of the systems

Formulation A

$$\sum_{j=1}^q \frac{\partial \psi(u_j)}{\partial \theta} (\psi(u_j) - \psi_n(u_j)) w_j = 0, \quad (4)$$

or

Formulation B

$$\sum_{j=1}^q \sum_{k=1}^q \frac{\partial \psi(u_j)}{\partial \theta} K^{jk} (\psi(u_k) - \psi_n(u_k)) w_j w_k = 0, \quad (5)$$

for $\theta = \alpha, \beta, \sigma, \mu$. The grid $\{u_j | j=1, \dots, q\}$ is symmetric about zero but does not include the origin, and K^{jk} denotes the j,k element of the inverse matrix $(K_{jk})^{-1}$, where

$$\begin{aligned} K_{jk} &= n \operatorname{cov}(\psi_n(u_j), \psi_n(u_k)) \\ &= \operatorname{Re} \phi(u_j - u_k) + \operatorname{Im} \phi(u_j + u_k) - \psi(u_j) \psi(u_k). \end{aligned} \quad (6)$$

The weights $\{w_j | j=1, \dots, q\}$ also depend on the parameters $\alpha, \beta, \sigma, \mu$, and are described in the Numerical Method section. Both Formulations A and B represent modified, weighted χ^2 minimum procedures, corresponding to the respective objective functions

$$A: S_n = \sum_{j=1}^q (\psi(u_j) - \psi_n(u_j))^2 w_j, \quad (7)$$

$$B: Q_n = \sum_{j=1}^q \sum_{k=1}^q (\psi(u_j) - \psi_n(u_j)) w_j K^{jk} w_k (\psi(u_k) - \psi_n(u_k)). \quad (8)$$

The following points are critical for practical application:

- 1) The shapes of ψ and ψ_n are highly dependent on location and scale parameters, and so should be standardized;
- 2) The estimators are improved by making the gridpoints and weights depend on α and β ;

- 3) Since the procedures are adaptive ($\{u_j\}$, $\{w_j\}$ and $\{K_{jk}\}$ depend on unknown parameters), algorithms must be iterative;
- 4) Since α , β and σ are always constrained, each iteration involves solution of a nonlinear optimization problem with variable bound constraints.

Our procedures may therefore be summarized as follows, where a tilde indicates estimators, their values, or adaptively standardized quantities.

Begin with initial guesses for the parameters. At each iteration, compute and save $\{u_j\}$, $\{w_j\}$, possibly $\{K^{jk}\}$, and standardized empirical characteristic function values $\{\tilde{\psi}_n(u_j)\}$, based on the latest $(\tilde{\alpha}, \tilde{\beta})$. The objective S_n or Q_n is then minimized (an "optimization subproblem"), and cumulative location and scale estimates (\tilde{l}, \tilde{s}) are updated. Iteration stops when values of σ and μ minimizing S_n or Q_n are acceptably close to unity and zero, respectively.

Estimators whose values are not on a bound are asymptotically multivariate Gaussian distributed. The asymptotic covariance matrices $\{\Sigma_i\}$ of the estimators are derived in Paulson and Delehanty (1982). The basic formula is

$$\Sigma_i = H_i^{-1} V_i H_i^{-1}, \quad i = A, B. \quad (9)$$

There are two particularly appealing ways to approximate $\{\Sigma_i\}$. In "approximation (i)", expectations are approximated from the data: H is computed by differencing the objective at the final optimum, and

$$V_A = 4D^T K D, \quad (10)$$

$$V_B = 4D^T K^{-1} K^{(w)} K^{-1} D. \quad (11)$$

Here

$$D_{j\theta} = \frac{\partial \tilde{\psi}(u_j)}{\partial \theta} w_j, \quad (12)$$

θ ranging over the parameters free of bounds,

$$\tilde{K}_{jk} = n^{-1} \sum_{m=1}^n (\tilde{\psi}(u_j) - \cos u_j \bar{x}_m - \sin u_j \bar{x}_m)(\tilde{\psi}(u_k) - \cos u_k \bar{x}_m - \sin u_k \bar{x}_m), \quad (13)$$

and

$$\tilde{K}_{jk}^{(w)} = \tilde{K}_{jk} w_j w_k. \quad (14)$$

By location and scale invariance, $(\tilde{\sigma}, \tilde{\mu})$ are set to $(1, 0)$ during these computations, and \tilde{K} scaled. In "approximation (ii)", expectations are calculated analytically, so K replaces \tilde{K} in (10), (11), and (14), and factors of 2 are omitted. The expected Hessian has elements

$$H_{A\theta\theta'} = \sum_{j=1}^q \frac{\partial \tilde{\psi}(u_j)}{\partial \theta} \frac{\partial \tilde{\psi}(u_j)}{\partial \theta'} w_j, \quad (15)$$

$$H_{B\theta\theta'} = D^T K^{-1} D,$$

where θ and θ' range over free parameters.

To analyze domains of attraction, we use what we refer to as the k-sum procedure. If k is a positive integer, the power

$$\phi_n^k(u) = n^{-k} \sum_{j_1=1}^n \cdots \sum_{j_k=1}^n \exp(iu(x_{j_1} + \cdots + x_{j_k})) \quad (16)$$

is the characteristic function corresponding to the k^{th} convolution power of the empirical distribution function $F_n(x)$, and can be interpreted as empirical characteristic function of all possible k -sums $\{x_{j_1} + \cdots + x_{j_k}\}$, sampling with replacement from $F_n(x)$. We add real and imaginary parts and standardize, giving $\tilde{\psi}_n^k(u)$, say, and estimate $(\tilde{\alpha}_k, \tilde{\beta}_k, \tilde{\sigma}_k, \tilde{\mu}_k)$ for different values of k . If the sample distribution is

attracted to a stable law with parameters $(\alpha, \beta, \sigma, \mu)$, the sequence of normalized estimators $(\tilde{\alpha}_k, \tilde{\beta}_k, \tilde{\sigma}_k^{1/\tilde{\alpha}_k}, \tilde{\mu}_k/k)$, for reasonable values of k , should approach $(\alpha, \beta, \sigma, \mu)$. In particular, a rapid rise in $\{\tilde{\alpha}_k\}$ may indicate that a stable model is not appropriate, a possible alternative being a mixture of finite variance components with differing scale parameters.

The k-sum procedure can thus be used in a sensitivity analysis, to examine how well the data support the stability assumption. Other possible tools for sensitivity analysis are varying the mechanism (to be described below) underlying the weights $\{w_j\}$, and comparing approximations (i) and (ii) of the estimated asymptotic covariance matrix, provided n is large enough for approximation (i) to be accurate.

NUMERICAL METHOD

The main computational task required is solution of bound-constrained nonlinear optimization problems. Although Formulations A and B lead to nonlinear least squares problems, current algorithms for nonlinear least squares do not allow constraints (Hiebert, 1981). Numerical Algorithms Group (NAG) subroutine E04KBF (NAG, 1981) is used for optimization. E04KBF is a quasi-Newton procedure, requiring an objective function and analytical first partial derivatives. It is substantially faster than the gradient projection routine used by Paulson, Holcomb and Leitch (1975), although the latter is very reliable. The other complicated numerical procedure required is inversion of a positive definite symmetric matrix (K , H or \tilde{H}), for which NAG subroutine F01ABF is used. Various NAG utility procedures are also used, see Auxiliary Algorithms. The use of NAG

procedures inhibits transportability in that the algorithm, as presented, is only usable at installations having the NAG Library. However, listings of rapid, high-quality algorithms for constrained optimization have not appeared in the literature (see Chambers, 1977, pp. 159-160; the situation described there has not improved). Given that E04KBF is used, reliance on additional NAG Library procedures is expedient.

We require a minimum of $q=20$ gridpoints $\{u_j\}$, and prefer $q=20$ or 40, since they are reasonable values in practice, and have been tested extensively. Only the positive gridpoints are explicitly required, due to symmetry of the grid and the Hermitian property of characteristic functions. They are computed as follows: An endpoint U is chosen as $3, \tilde{\alpha} \geq 1.8; 3.3, 1.8 > \tilde{\alpha} \geq 1.7; 3.6, 1.7 > \tilde{\alpha} > 1; 5, \tilde{\alpha}=1; 4, 1 > \tilde{\alpha} \geq .9; 5, .9 > \tilde{\alpha} \geq .8; 7, .8 > \tilde{\alpha} \geq .6; 10, \tilde{\alpha} < .6$. An inner number I of points is selected close to the origin: $I=2$ if $q<30$ and 3 if $q \geq 30$, 1 being subtracted if $\tilde{\alpha} \leq .5$. The inner I points are spaced as follows: if $\tilde{\alpha} > 1$, $\frac{1}{2}$ the "a-optimal" values of Feuerverger and McDunnough (1981b) for the nearest (larger) a are used; if $\tilde{\alpha} \leq 1$, the first I points giving $q/2$ equal increments of $\log(u + a^{*3})$ between 0 and U are multiplied by $\frac{1}{2} a^{*2}$ ($a^{*} = \max(\tilde{\alpha}, .3)$). The remaining points are logarithmically spaced out to U : if $\tilde{\alpha} > 1$, the function $\log(1 + u/2)$ is used, and if $\tilde{\alpha} \leq 1$, $\log(u + a^{*3})$ is used. This rather complicated ad hoc scheme was developed through graphical inspection of $\psi(u)$ and $\psi_n(u)$, comparisons of asymptotic efficiencies, and parameter estimation for real and simulated data. No claims of optimality are made, but the scheme provides high efficiencies if efficiency is preferred, or good matches between ψ and ψ_n if curve fitting is preferred. The point of stratified and logarithmic spacing is

to emphasize u values near the origin. Details when $\alpha \leq 1$ reflect the fact that $\psi(u)$ has a sharp cusp near the origin, but decays slowly. The stepwise nature of the scheme is not deemed a serious drawback.

The weights $\{w_j\}$ are computed as follows:

Under Formulation A,

$$w_j = \frac{|\phi(u_j)|^{2\lambda}}{K_\tau(u_j, u_j)} = \frac{\exp(-2\lambda|u_j|^\alpha)}{K_\tau(u_j, u_j)}, \quad (17)$$

and under Formulation B,

$$w_j = |\phi(u_j)|^\lambda = \exp(-\lambda|u_j|^\alpha), \quad (18)$$

where λ and τ are supplied by the user, $0 \leq \tau \leq 1$,

$$K_\tau(u, u) = 1 + \tau(\operatorname{Im} \tilde{\phi}(2u) - \tilde{\psi}^2(u)), \quad (19)$$

and λ is recommended nonnegative. Rationale for these weights, and some corresponding asymptotic efficiencies, are in Paulson and Delehanty (1982). We recommend $\tau=1$ under Formulation A. Under Formulation B, it is convenient to let $\tau \geq 0$ represent a fraction of the average diagonal element by which to inflate K , giving a matrix we shall call A . We have only found this inflation necessary if α is very close to two, when $\tau=0.01$ suffices.

To use the quantity λ as a tool for sensitivity analysis, we interpret it as a damping factor, lessening the effects of noise in $\tilde{\psi}_n(u)$ for larger $|u|$. If the data are truly stable and the sample size is fairly large (say 150 or more), estimates should change little as λ varies, say, from 0 to 1. Large discrepancies in the estimates for different values of λ indicate problems with the data or the stable assumption or both. It may not be easy to isolate the difficulty but further study is

definitely required.

For the k-sum procedure, $k > 1$, the situation regarding gridpoints and weights changes. Tests so far indicate that when $\alpha > 1$, Formulation A, with gridpoints equispaced from 0 to U, gives better results than "efficient configurations" used for $k=1$. Reasons for this are unclear. A possible explanation is that when $\alpha > 1$ and $k > 1$, $\tilde{\psi}_n^k(u)$ is so smooth that estimation is practically equivalent to deterministic curve fitting, and implicit or explicit emphasis on gridpoints near the origin neglects important curvature for large $|u|$. Accordingly, when $k > 1$ and $\alpha > 1$, we equispace gridpoints and set all weights to 1. When $\alpha \leq 1$, $\tilde{\psi}_n^k(u)$ has a sharp cusp near the origin and remains a jagged curve as k increases, due to the presence of very large observations. In this situation, we set all weights to 1 and use basically the same gridpoint scheme as when $k=1$, omitting only multiplication of the inner points by $\alpha^{*2}/4$. In either case, Formulation A is recommended.

An important question is how large k may be taken. Equation (16) suggests that we cannot expect to take k arbitrarily large. There seems to be a tendency for α to increase and β to drift if k is too large, though this may be partially due to suboptimal gridpoints or weighting. It appears that when n is large, say 500 or more, k may safely be taken up to 20. Care is required for smaller n , and when α is small or very near two.

Implicit standardization is carried out as follows. Let k be a positive integer, and (\hat{l}, \hat{s}) cumulative location and scale estimates.

Then

$$\tilde{\psi}_n^k(u_j) = \rho_{jk}(\cos \gamma_{jk} + \sin \gamma_{jk}), \quad (20)$$

where

$$\rho_{jk} = |\phi_n(u_j/\tilde{s})|^k \quad (21)$$

and

$$\gamma_{jk} = k \arg \phi_n(u_j/\tilde{s}) - \tilde{\ell} u_j/\tilde{s}. \quad (22)$$

No problems of principal values arise, and complex arithmetic is not used. The FORTRAN mathematical library function ATAN2 computes arguments.

The estimator \tilde{a} may be bounded in (closed) subintervals of $[\delta, 1-\epsilon]$, $[1, 1]$, or $[1+\epsilon, 2]$ unless $\tilde{\beta}$ is fixed at 0, when $[\delta, 2]$ is possible (δ and ϵ are small positive numbers), while $\tilde{\beta}$ may be bounded in subintervals of $[-1, 1]$. Estimators $\tilde{\sigma}$ and $\tilde{\mu}$ may be constrained arbitrarily in $[\delta, \infty)$ and $(-\infty, \infty)$, respectively, unless \tilde{a} is fixed at 1 and $\tilde{\beta}$ is not fixed at 0, when $\tilde{\mu}$ cannot be constrained. Bounds on σ and μ are internally set for use in subproblems. These bounds must be wide enough to allow the "true values" to be found, but narrow enough to deter straying into undesirable regions, particularly $\sigma \rightarrow \infty$, $|\mu| \rightarrow \infty$. The ad hoc bounds of $[-5, 5]$ for μ and $[0.2, 5]$ for σ work well in practice. If $\tilde{\sigma}$ or $\tilde{\mu}$ are initially constrained, their internal bounds are adaptively modified, see the Algorithm for description.

Initial guesses for the parameters are required. We do not find their specification particularly important, provided \tilde{a} is on the correct side of 1 in the nonsymmetric case. We have used the median and semi-interquartile range as guesses for $\tilde{\mu}$ and $\tilde{\sigma}$, and averages of upper and lower bounds for \tilde{a} and $\tilde{\beta}$. If \tilde{a} is anticipated less than 1.2, say, it is

worthwhile to put more effort into initial guesses, since fewer iterations will be required (the semi-interquartile range will overestimate σ , and if α is near but different from 1, the median is nearer $\mu - \frac{2}{\pi} \beta \sigma \log \sigma$ than μ).

Convergence is judged by a tolerance on subproblem solutions, $\max(|\sigma^{(m)} - \bar{\sigma}|, |\mu^{(m)} - \bar{\mu}|)$, (or $\max(|\alpha^{(m)} - \bar{\alpha}|, |\beta^{(m)} - \bar{\beta}|)$ if $\bar{\alpha}$ and $\bar{\beta}$ are fixed), with a maximum allowable number of iterations. Attainable tolerances depend on n , but more strongly on the underlying parameters. If $\bar{\alpha}$ is near two, $\tilde{\psi}_n$ is very smooth and stringent tolerances such as 10^{-6} may be attained. If $\bar{\alpha} \leq 1.2$, $\tilde{\psi}_n$ has many small oscillations due to large observations, and, especially for smaller samples, it may be preferable to terminate after a fixed number of iterations. Good estimates are generally obtained within five iterations, fewer if initial guesses are good; if stringent tolerances are required, or for difficult problems (skewed distributions with $0.9 \leq \alpha \leq 1.1$) more may be required. Convergence is typically slower under Formulation B, since the weighting mechanism is more complicated.

Approximation of asymptotic covariance matrices requires little description. We note that for approximation (i) and the q values we use, it is faster to define a vector

$$\delta_j^T = (\tilde{\psi}(u_1) - \cos u_1 \tilde{x}_j - \sin u_1 \tilde{x}_j, \dots, \tilde{\psi}(u_q) - \cos u_q \tilde{x}_j - \sin u_q \tilde{x}_j), \quad (23)$$

and cumulate

$$\tilde{y} = 4n^{-1} \sum_{j=1}^n (\delta_j^T \delta_j) (\delta_j^T \delta_j)^T \quad (24)$$

under Formulation A, or

$$\tilde{Y} = 4n^{-1} \sum_{j=1}^n (\underline{D}^T \underline{A}^{-1} \delta_j) (\underline{D}^T \underline{A}^{-1} \delta_j)^T \quad (25)$$

under Formulation B, than to cumulate \tilde{K} . The matrix \underline{D} is computed by the function/gradient subroutine. E04KBF returns an approximate Hessian, which could conceivably be used for \tilde{H} in approximation (i). Rather often, however, E04KBF will terminate with its failure indicator set to 3 and the Hessian set to the identity matrix, even though the optimum may be reliable. It is therefore simpler to compute \tilde{H} by differencing. The following procedures is used: Set an initial Hessian to 0, and the steplength to 10^{-3} . Successively divide the steplength by $\sqrt{10}$ and approximate the Hessian by differencing; three-point differencing for the diagonal, and four-point for off-diagonal elements. Compare elements of successive approximations by maximum relative or absolute differences, according as the element of the latest approximation exceeds 1 in absolute value or not. A tolerance of 10^{-6} is used for this convergence criterion. If convergence has not occurred with a steplength of 10^{-5} , the result with steplength 10^{-4} is used.

Approximation (i) of the asymptotic covariance matrix is rather expensive to compute. It should not be computed for smaller sample sizes, as it implicitly involves estimation of $\frac{1}{2}q(\frac{1}{2}q+1)$ covariances.

Following is an informal description, in Algorithm form, of the basic routine STABLE. Approximate asymptotic covariance matrices may also be computed, but this presents no logical difficulties, so is omitted.

Algorithm

Produces estimates $(\tilde{\alpha}, \tilde{\beta}, \tilde{\sigma}, \tilde{\mu})$ for k-sums ($k \geq 1$), based on a sample (x_1, \dots, x_n) .

Input parameters: $k, n, \{x_j\}, q, \lambda, \tau$, Formulation (A or B), convergence tolerance ϵ , maximum number M of iterations, and flags whether $\tilde{\sigma}$ and $\tilde{\mu}$ are constrained.

Input/output parameters: $(\tilde{\alpha}, \tilde{\beta}, \tilde{\sigma}, \tilde{\mu})$ are initial guesses on entry and estimates on exit, $(\alpha_L, \beta_L, \sigma_L, \mu_L)$ and $(\alpha_u, \beta_u, \sigma_u, \mu_u)$ are lower bounds. The (σ, μ) bounds are changed, but restored on exit. In the special case where $\tilde{\alpha}$ is fixed at 1, $\tilde{\mu}$, on entry, is the initial guess for location $\mu + \frac{2}{\pi} \beta \sigma \log \alpha$.

Auxiliary quantities \tilde{l} and \tilde{s} are cumulative location and scale estimates. Entry values of $(\sigma_L, \sigma_u, \mu_L, \mu_u)$ are stored in (b_1, b_2, b_3, b_4) . On entry and exit, $(\tilde{\sigma}, \tilde{\mu}, \sigma_L, \mu_L, \sigma_u, \mu_u)$ are normalized.

S1 [Initialize.]

Set $\tilde{l} \leftarrow k \bar{u}$, $\tilde{s} \leftarrow k^{1/\tilde{\alpha}} \tilde{\sigma}$, $m \leftarrow 0$.

Save $(b_1, b_2, b_3, b_4) \leftarrow (\sigma_L, \sigma_u, \mu_L, \mu_u)$.

if $\tilde{\mu}$ is unconstrained then set $\mu_L \leftarrow -5$, $\mu_u \leftarrow 5$;

else if $\tilde{\mu}$ is fixed then set $\mu_L \leftarrow \mu_u \leftarrow 0$;

else set $\mu_L \leftarrow k \mu_L$, $\mu_u \leftarrow k \mu_u$.

if $\tilde{\sigma}$ is unconstrained then set $\sigma_L \leftarrow 0.2$, $\sigma_u \leftarrow 5$;

else if $\tilde{\sigma}$ is fixed then set $\sigma_L \leftarrow \sigma_u \leftarrow 1$;

else set $\sigma_L \leftarrow k^{1/\tilde{\alpha}} \sigma_L$, $\sigma_u \leftarrow k^{1/\tilde{\alpha}} \sigma_u$.

S2 [Looping point for iteration; save adaptive quantities for subproblem.]

Increment $m \leftarrow m + 1$.

Save $\tilde{\alpha}^{(m-1)} \leftarrow \tilde{\alpha}$, $\tilde{\beta}^{(m-1)} \leftarrow \tilde{\beta}$.

if $\tilde{\sigma}$ is constrained but not fixed then set $\sigma_L \leftarrow \max(0.2, b_1/\tilde{s})$,

$\sigma_u \leftarrow \min(5, b_2/\tilde{s})$.

if $\tilde{\mu}$ is constrained but not fixed then set $\mu_L \leftarrow \max(-5, (b_3 - \tilde{\ell})/\tilde{s})$,

$\mu_u \leftarrow \min(5, (b_4 - \tilde{\ell})/\tilde{s})$.

Set $\tilde{\sigma} \leftarrow 1$, $\tilde{\mu} \leftarrow 0$.

Compute and save positive gridpoints $\{u_j \mid j = q/2+1, \dots, q\}$,

weights $\{w_j \mid j = 1, \dots, q\}$, and standardized empirical characteristic function values $\{\tilde{\psi}_n^k(u_j) \mid j = 1, \dots, q\}$.

if Formulation B then compute and invert A.

S3 [Subproblem.]

Solve the optimization problem

$$\min \sum_{j=1}^q (\psi(u_j) - \tilde{\psi}_n^k(u_j))^2 w_j \quad (\text{Formulation A})$$

or

$$\min \sum_{i=1}^q \sum_{j=1}^q w_i (\psi(u_i) - \tilde{\psi}_n^k(u_i)) A^{ij} (\psi(u_j) - \tilde{\psi}_n^k(u_j)) w_j \quad (\text{Formulation B}),$$

yielding new $(\tilde{\alpha}, \tilde{\beta}, \tilde{\sigma}, \tilde{\mu})$.

S4 [Update and test convergence.]

Set $\tilde{\ell} \leftarrow \tilde{\ell} + \tilde{s} \tilde{\sigma}$.

if $\tilde{\alpha}=1$ then set $\tilde{\ell} \leftarrow \tilde{\ell} + \frac{2}{\pi} \tilde{s} \tilde{\beta} \tilde{\sigma} \log \tilde{\sigma}$.

Set $\tilde{s} \leftarrow s \tilde{\sigma}$.

if $\tilde{\sigma}$ and \tilde{u} are fixed then error $\leftarrow \max(|\tilde{\alpha}-\alpha^{(m-1)}|, |\tilde{\beta}-\beta^{(m-1)}|)$;

else error $\leftarrow \max(|\tilde{\sigma}-1|, |\tilde{u}|)$.

if error $\geq \epsilon$ and $m < M$ then go to S2.

S5 [Final estimates.]

Set $(\sigma_L, \sigma_u, \mu_L, \mu_u) \leftarrow (b_1, b_2, b_3, b_4)$.

if $\tilde{\alpha}=1$ then set $\tilde{\ell} \leftarrow \tilde{\ell} - \frac{2}{\pi} \tilde{\beta} \tilde{s} \log \tilde{s}$.

Set $\tilde{u} \leftarrow \tilde{\ell}/k$, $\tilde{\sigma} \leftarrow \tilde{s}/k^{1/\tilde{\alpha}}$.

STRUCTURE

SUBROUTINE STABLE (X,N,MODE,KSUM,XLAM,TAU,NPTS,TOL,MAXIT,XL,XH,NPAR,
ISCLBD,LOCBND,ICOV,VCV1,VCV2,WORK,LWORK,IWORK,LIWORK,IAUTL)

Formal parameters

X	Real array (N)	input:	sample
N	Integer	input:	sample size
MODE	Integer	input:	formulation; if zero, then Formulation B is used, else Formulation A
KSUM	Integer	input:	convolution power k
XLAM	Real	input:	λ
TAU	Real	input:	τ
NPTS	Integer	input:	q
TOL	Real	input:	convergence tolerance
MAXIT	Integer	input:	maximum allowable number of iterations
XL	Real array (NPAR)	input:	lower bounds for parameters ($\alpha, \beta, \sigma, \mu$); the third and fourth elements change during execution
		output:	input values are restored
XH	Real array (NPAR)	input:	upper bounds for parameters; the third and fourth elements change during execution
		output:	input values are restored
NPAR	Integer	input:	number of parameters (4)
ISCLBD	Integer	input:	flag if σ is constrained: if negative, σ is fixed at $XB(3)$; if zero, σ is free to vary and initial values of $XL(3)$ and $XH(3)$ are irrele- vant; if positive, σ is constrained in $[XL(3), XH(3)]$

LOCBND Integer	input:	flag if \bar{u} is constrained: if negative, \bar{u} is fixed at XB(4); if zero, \bar{u} is free to vary and initial values of XL(4) and XH(4) are irrelevant; if positive, \bar{u} is constrained in [XL(4),XH(4)]
ICOV Integer	input:	flag for computation of covariance matrices: if negative, neither approximation (i) nor (ii) is computed; if zero, both approximations are computed; if positive, only approximation (ii) is computed
VCV1 Real array(NPAR,NPAR) output:		covariance matrix approximation (i) if requested; the strict lower triangle contains correlations, the upper triangle contains covariances (times n); if a parameter is on a bound, the corresponding elements are zero
VCV2 Real array(NPAR,NPAR) output:		covariance matrix approximation (ii) if requested; the strict lower triangle contains correlations, the upper triangle covariances (times n); if a parameter is on a bound, the corresponding elements are zero
WORK Real array (LWORK)	workspace:	
	output:	some elements may be of interest on output (see Restrictions)
LWORK Integer	input:	
IWORK Integer array(LIWORK)	workspace:	
	output:	some elements may be of interest on output (see Restrictions)
LIWORK Integer	input:	
IVNIT Integer	input:	if positive, unit number for output (see Additional Comments); if zero or negative, no output is produced
IFault Integer	output:	failure indicator

Failure indicators

IFAULT = 0 indicates success. Nonzero values of IFAULT are due to two types of errors. The first type is input errors, detected in STABLE; IFAULT will be

```

1   if MAXIT<0;
2   if N<50 (see Restrictions);
3   if KSUM <= 0;
4   if T<0 or T>1 and MODE<0;
5   if NPTS<20 or mod(NPTS,2)<0;
6   if TOL<0;
7   if NPAR<4;
8   if insufficient workspace was allotted (see Restrictions);
9   if improper bounds were supplied. The following conditions
cause this failure:
XL(i)>XB(i) or XL(i)>XH(i) or XB(i)>XH(i), i=1,2
XL(1)<0 or XH(1)>2
XL(1)<-1 or XH(1)>1
(XL(2)<0 or XH(2)<0) and (XL(1)<1 and XH(1)>1
or XL(1)<1 and XH(1)>1)
XB(3)<0
ISCLBD<0 and (XL(3)>XB(3) or XL(3)>XH(3) or XB(3)>XH(3))
ISCLBD<0 and XL(3)<XH(3)
LOCBND<0 and (XL(4)>XB(4) or XL(4)>XH(4) or XB(4)>XH(4))
LOCBND<0 and XL(4)<XH(4)
LOCBND<0 and XL(1)=XH(1)=1 and (XL(2)<0 or XH(2)<0).

```

On input errors, STABLE terminates immediately, without performing any computations. The second type of error occurs after some computation.

IFAULT will be

```

10  if A was found numerically non positive definite;
11  if A was found ill-conditioned;
12  if too many function evaluations were required during solution
of a subproblem;
13  if iteration converged, but
the most recent E04KBF fault indicator was 3 and
internal checks were not met. These checks are
(i)  $\|G\|^2 < 10 * X02AAF(DUMMY)$ , and
(ii)  $K < 1/\|G\|$ , as recommended by E04KBF
documentation, where  $\|G\|$  is the norm of the projected
gradient and K the estimated condition number of the
projected Hessian matrix;

```

- 14 if there were repeated problems with overflow in the Cholesky factors of the projected Hessian;
- 15 if iteration converged, but the most recent E04KBF fault indicator was 5 and internal checks were not met;
- 16 if convergence did not occur in MAXIT iterations;
- 17 if convergence did not occur in MAXIT iterations, the most recent E04KBF fault indicator was 3, and internal checks were not met;
- 18 if convergence did not occur in MAXIT iterations, the most recent E04KBF fault indicator was 5, and internal checks were not met.

Conditions IFAULT=10 and 11 are detected in SETECF (they are caused by τ being too small under Formulation B), the remainder in STABLE.

IWORK(2) and IWORK(3) (see Restrictions) are failure indicators for asymptotic covariance matrix versions (i) and (ii) respectively. Zero indicates success, 1 that H was non positive definite, and 2 that H was ill-conditioned, the failures detected in SETVCV. If IFAULT=1-12 or 14, covariance matrices are not computed, and their fault indicators are set to the corresponding value of IFAULT.

Auxiliary algorithms

The user has only to call STABLE. Auxiliary procedures fall into two groups: those supplied here, and NAG Library procedures. The following subroutines are supplied:

SUBROUTINE GRIDWT(PAR,NPAR,XLAM,TAU,PTS,NPTS2,WT,NPTS,MODE,KSUM): computes gridpoints and weights;

SUBROUTINE CHARFN(U,PAR,NPAR,RE,XIM): computes real and imaginary parts of standard stable characteristic function $\phi(u)$;

SUBROUTINE FUNCT(IFLAG,N,XC,FC,GC,IW,LIW,W,LW): objective function/gradient evaluation;

SUBROUTINE SETECF(X,N,PAR,NPAR,MODE,TAU,SIGMA,XMU,KSUM,IA,NPTS2,NPTS,
 PTS,ECF,A,AINV,WORK,IFault): computes standardized empirical characteristic function values $\tilde{\psi}_n^k(u)$, computes and inverts A under Formulation B;

SUBROUTINE MONIT(N,XC,FC,GC,ISTATE,GPJNRM,COND,POSDEF,NITER,NF,IW,LIW,
 W,LW): monitors the progress of E04KBF;

SUBROUTINE VARIAB(ICOV,X,N,PAR,NPAR,MODE,SIGMA,XMU,ISUB,NVAR,PTS,NPTS2,
 WT,ECF,NPTS,DERIV,WORK,HOLD,A,IA,AINV,VCV1,VCV2,H,NVAR1,V,IW,LIW,W,LW,
 IFAIL1,IFAIL2): computes approximate asymptotic covariance matrices;

SUBROUTINE VMATRX (X,N,MODE,XMU,SIGMA,PTS,NPTS2,WT,ECF,WORK,NPTS,DERIV,
 V,HOLD,NVAR): computes \hat{Y} for version (i) of asymptotic covariance matrix;

SUBROUTINE DAPROD(FAC1,IFAC1,NPTS,FAC2,WORK,NVAR): auxiliary matrix multiplication for VARIAB;

SUBROUTINE HVPROD(FAC1,IFAC1,NVAR,FAC2,NPTS,VH,IVH): auxiliary matrix multiplication for VARIAB;

SUBROUTINE SETVCV(ISUB,NVAR,H,NVAR1,V,WORK,VCV,NPAR,SIGMA,IFault): auxiliary routine for VARIAB;

SUBROUTINE HESDIF(PAR,NPAR,ISUB,H,SAVE1,SAVE2,NVAR,IW,LIW,W,LW): computes an approximate Hessian by differencing for version (i) of asymptotic covariance matrix.

The following NAG Library procedures are used:

REAL FUNCTION X02AAF(DUMMY): returns the smallest positive ϵ such that $1.0 + \epsilon > 1.0$;

SUBROUTINE E04KBF(N,FUNCT,MONIT,IPRINT,LOC SCH,INTYPE,MINLIN,MAXCAL,ETA,
 XTOL,STEPMX,FEST,IBOUND,BL,BU,X,HESL,LH,HESD,ISTATE,F,G,IW,LIW,W,LW,IFAIL): solves optimization problems. Control parameters are set as follows:

```

IPRINT = 0
LOC SCH = .TRUE.
INTYPE = 3 for subproblems after the first if parameters which are
        not fixed are not on bounds, else 0
MINLIN = NAG Library routine E04LBS
MAXCAL = 400
ETA = 0.9
XTOL = 10.0 $\sqrt{X02AAF(DUMMY)}$  explicitly, so it is available on exit
STEPMX = 0.25
FEST = 0.0
IBOUND = 0 ;
  
```

SUBROUTINE F01ABF(A,IA,N,B,IB,Z,IFAIL): inverts the positive definite symmetric matrix A;

SUBROUTINE F01CAF(A,M,N,IFAIL): sets matrix A to zero;

SUBROUTINE F01CMF(A,LA,B,LB,M,N): copies elements of matrix A into matrix B;

SUBROUTINE F01CKF(A,B,C,N,IP,M,Z,IZ,IOP,T,IFAIL): matrix multiplication $A=BC$, where B or C may be overwritten.

RESTRICTIONS

We require the sample size N at least 50, since for smaller samples $\tilde{\psi}_n(u)$ is not generally sufficiently smooth to allow accurate estimation. Since $\tilde{\alpha}$ and $\tilde{\beta}$ are bounded in the narrow ranges $(0,2]$ and $[-1,1]$ and have standard errors decreasing as $N^{-\frac{1}{2}}$, it is preferable to have $N \geq 100$. For N less than 150, say, relatively large values of λ may be preferred, to damp out noise in $\tilde{\psi}_n(u)$. We further require $NPTS \geq 20$.

Extended work vectors WORK and IWORK are required, in order to communicate information to FUNCT and MONIT without using COMMON blocks. To aid readers who may wish to adapt the algorithm to installations not having the NAG Library, we describe the use of these work vectors.

The required length of WORK is $10 + 11*NPAR + NPAR*(NPAR-1)/2 + (3+NPAR)*NPTS + NPTS + NPTS/2$ if $MODE \neq 0$, with an additional $NPTS*(2*NPTS+1)$ required if $MODE=0$. Some sample lengths are

<u>MODE</u>	<u>NPTS=20</u>	<u>NPTS=40</u>
0	1030	3600
nonzero	210	360

The subvector W is passed to E04KBF, FUNCT, and MONIT.

The required length of IWORK is $7 + NPAR$. The subvector IW is passed to E04KBF, FUNCT, and MONIT.

<u>IWORK starting point</u>	<u>IW starting point</u>	<u>Elements</u>	<u>Use for</u>
1	-	1	Iteration count
2	-	NPAR	ISTATE vector for E04KBF, workspace for VARIAB.
(other addresses internally computed)			If covariance matrices are requested, on exit IWORK(2) contains a fault indicator for approximation (i), IWORK(3) contains a fault indicator for approximation (ii), and IWORK(4) contains the number of iterations required to compute the approximate Hessian for approximation (i)
		2	Workspace for E04KBF, HESDIF
	1	1	Stores MODE
	1	1	Stores output unit number IUNIT
	1	1	Stores NPTS
	1	1	Stores 1 less than the address of PTS(1) in W

PRECISION

Double precision will be required on computers with 32 bit wordlength.

The precision used by the local NAG Library implementation should be adequate. To change the precision:

- change all REAL declarations to DOUBLE PRECISION;
- replace constants by double precision versions, constants $\frac{\pi}{2}$, $\frac{2}{\pi}$, $\sqrt{10}$ typed in to machine accuracy;
- declare NAG Library function X02AAF as DOUBLE PRECISION;
- change the precision of FORTRAN library functions, i.e., ABS to DABS, ATAN2 to DATAN2, SIGN to DSIGN, etc. FLOAT(I) can be replaced by DBLE(FLOAT(I)).

If extremely large observations are present in the sample, there may be a loss of significant figures when computing sines and cosines in SETECF and VMATRIX. This should not occur when real data is used, but can be a problem with simulated data for small α .

TIME

Execution times depend on the quality of initial guesses and properties of the real data used, and vary somewhat throughout the parameter space. As a rough guide, we give some statistics for simulated data, using a moderately difficult situation with $\alpha > 1$. Tables 1a and 1b provide approximate running times for Formulation A, $q=40$, and Formulation B, $q=20$, $n=100, 200, 500, 1000, 2500$. Timing starts upon entry to STABLE. Samples from $S(1.3, -.5, 3, 15)$ were generated using the method of Chambers, Mallows, and Stuck (1976). Initial guesses for $\alpha, \beta, \sigma, \mu$ in all cases were $1505 = \frac{1}{2}(1.01+2)$, 0, $\frac{1}{2}(x_{.75} - x_{.25})$, and $x_{.5}$, the sample median, respectively. Because of skewness, the median is not a good estimator of μ in this case. Five iterations were used. Time required to compute asymptotic covariance matrices includes approximations (i) and (ii), except where noted. Timings are for a double precision version of the algorithm, compiled by the IBM FORTRAN H Extended compiler, and run on an IBM 370/3033.

The following qualitative points are clear from this rather restricted set of timings. There is a substantial overhead, which may crudely be assumed fixed, associated with nonlinear optimization, although E04KBF solves the optimization subproblems rapidly. For large samples, run time is dominated by evaluation of the empirical characteristic function, and thus is asymptotically linear in n for a fixed number of iterations.

Table 1a

Timings for Formulation A, q=40, on Simulated Samples
from $s(1.3, -.5, 3, 15)$; $\lambda=1$ for $n \leq 200$ and .5 for $n > 200$, $\tau=1$

<u>n</u>	<u>Iterations</u>	<u>Estimation time (sec)</u>	<u>Convergence criterion</u>	<u>Covariance matrix time</u>
100	5	0.7	5.4(-4)	0.1*
200	5	1.0	2.3(-2)	0.1*
500	5	1.8	1.8(-4)	0.8
1000	5	3.2	3.3(-5)	1.2
2500	5	7.5	4.8(-6)	2.5

*Sample size too small to compute approximation (i), only approximation (ii) computed.

Table 1b

Timings for Formulation B, q=20, on Simulated Samples
from $s(1.3, -.5, 3, 15)$; $\lambda=\tau=0$

<u>n</u>	<u>Iterations</u>	<u>Estimation time (sec)</u>	<u>Convergence criterion</u>	<u>Covariance matrix time</u>
100	5	0.9	1.2(-2)	0.3
200	5	1.2	3.2(-2)	0.4
500	5	1.6	1.8(-4)	0.5
1000	5	2.3	5.7(-5)	0.7
2500	5	4.4	1.5(-4)	1.4

Approximation (ii) of the asymptotic covariance matrix is quite easy to compute, while approximation (i) is highly time-consuming.

For fixed $k > 1$ with the k-sum procedure, one iteration generally suffices, provided estimates from the nearest value of k are used, and the estimates don't change much. For mixtures of very different distributions, or if the exponent $\tilde{\alpha}$ is near unity, more are required.

ADDITIONAL COMMENTS

Although output need not be produced, we recommend calling STABLE with IUNIT>0, so the user will have a record of how estimation progressed. The following information will then be printed out:

by MONIT: number of E04KBF iterations and function evaluations, objective function value, norm of projected gradient, subproblem solution, projected gradient, and estimated condition number of projected Hessian;

by STABLE: E04KBF fault indicator, and value of convergence criterion;

by HESDIF(if called): number of iterations needed to compute approximate Hessian, and steplength used.

Use of STABLE in "batch mode" has drawbacks. For instance, most faults arising in E04KBF are not diagnosed until iteration ceases. In practice, such faults may likely be due to the initial $\tilde{\alpha}$ being on the wrong side of 1. Further, when $\tilde{\alpha}$ is small, convergence tolerances are difficult to interpret, and the user may prefer direct control of iteration. We therefore prefer to use STABLE interactively, a copy of the output described above being directed to the terminal, and the user deciding after each iteration whether he wishes to continue. Required modifications are simple.

Faster and/or more compact codings of the Algorithm are possible, for instance, if β is known to be zero, if only Formulation A or Formulation B is desired, or if asymptotic covariance matrices are not desired. Generality is achieved at a price in efficiency.

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```

C*****CENTRAL SUBROUTINE OF ESTIMATION PROCESS.          STAB 001
C      STAB 002
C      STAB 003
C      STAB 004
C      STAB 005
C      STAB 006
C      STAB 007
C      STAB 008
C      STAB 009
C      STAB 010
C      STAB 011
C      STAB 012
C      STAB 013
C      STAB 014
C      STAB 015
C      STAB 016
C      STAB 017
C      STAB 018
C      STAB 019
C      STAB 020
C      STAB 021
C      STAB 022
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C      STAB 029
C      STAB 030
C      STAB 031
C      STAB 032
C      STAB 033
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C      STAB 047
C      STAB 048
C      STAB 049
C      STAB 050
C      STAB 051
C      STAB 052
C      STAB 053
C      STAB 054
C      STAB 055
C      STAB 056
C      STAB 057
C      STAB 058
C      STAB 059
C      STAB 060

C      CALLS - GROUT, SETECF, VARIAB
C      CALLS - GRDMT VIA EXTERNAL STM - FUNCT, MONIT, E04LBS
C      PROCEDURES CALLED -
C      N.A.G. X02AAF (RETURNS MACHINE PRECISION) WITH BOUNDED
C      ED04KBF (QUASI-NEWTON OPTIMIZATION)
C      VARIABLES)
C
C      F01CAF (SETS A MATRIX TO ZERO).
C
C      SUBROUTINE STABLE(X, N, MODE, KSUM, XLAM, TAU, NPTS, TOL, MAXIT,
C      *XL, XB, XH, NPAR, ISCLBD, LOCBD, ICOV, VCV1, VCV2, WORK, LWORK,
C      *IWORK, LWORK, IUNIT, IFAULT)
C      EXTERNAL ROUTINES
C      EXTERNAL ED04BS, FUNCT, MONIT
C
C      ARGUMENTS
C      INTEGER N, MODE, KSUM, NPTS, MAXIT, NPAR, ISCLBD, LOCBD, ICOV,
C      *LWORK, IWORK, IWORK(LWORK), IUNIT, IFAULT
C      REAL X(N), XLAM, TAU, TOL, XL(NPAR), XB(NPAR),
C      *VCV1(NPAR, NPAR), VCV2(NPAR, NPAR), WORK(LWORK)
C
C      FUNCTION CALLED
C      REAL X02AAF
C
C      LOCAL SCALARS
C      SPECIFICALLY FOR ED04BF PARAMETERS -
C
C      LOGICAL LOCSC
C      INTEGER LW, LIW, MAXCAL, IBOUND, IPRINT, LHESL, INTYPE
C      REAL ETA, XTOL, STEPMX, FEST
C
C      SCRATCH VARIABLES, SUBSCRIPT INDICATORS, AND CONSTANTS -
C
C      INTEGER IND, IND1, I0VFLW, NPTS2, IA, NVAR, NPTS, NWT,
C      *MECF, MDERIV, MWORK, MA, MAINV, MHESD, MIW, MV,
C      REAL SIGMA, XNU, XK, ZERO, PT2, TWOPI, ONE, TWO, SQRT10, FIVE,
C      *TEN
C      DATA LOCSC, MAXCAL, IBOUND, IPRINT, ETA, STEPMX, FEST
C      */TRUE, 400, 0, 0, 0.9, 0.25, 0.0/
C      DATA ZERO, PI2, TWOPI, ONE, TWO, SQRT10, FIVE, TEN
C      */0.0, 0.2, 0.6366197724, 1.0, 2.0, 3.162277660, 5.0, 10.0/
C
C      ON INPUT ERRORS (IFault = 1 - 9), EXIT IMMEDIATELY.
C
C      IWORK(1) = 0
C      WORK(1) = ZERO
C      IFault = 1
C      IF (MAXIT .LE. 0) RETURN
C      IFault = 2
C      IF (IN .LT. 50) RETURN
C      IFault = 3
C      IF (KSUM .LE. 0) RETURN
C      IFault = 4
C      IF (TAU .LT. ZERO .OR. MODE .NE. 0 .AND. TAU .GT. ONE) RETURN
C      IFault = 5
C      IF (NPTS .LT. 20 .OR. MOD(NPTS,2) .NE. 0) RETURN
C      IFault = 6
C      IF (TOL .LE. ZERO) RETURN
C      IFault = 7
C      IF (INPAR .NE. 4) RETURN
C      IFault = 8
C      NPTS2 = NPTS / 2
C      LHESL = (NPAR*NPAR - NPAR) / 2
C      LW = 10 + 11 * NPAR + LHESL + (3 + NPAR) * NPTS + NPTS2
C      IF (MODE .EQ. 0) LW = LW + NPTS * (2*NPTS + 1)

```

```

C IF (LWORK .LT. LW .OR. LIWORK .LT. NPAR + 7) RETURN
C
C CHECKING OF PARAMETER BOUNDS (IFault = 9 IF WRONG)
C
C IF (FAULT = 9
C     IF (XL(1) .GT. XB(1) .OR. XL(1) .GT. XH(1) .OR. XB(1) .GT. XH(1)) STAB 061
C     IF (XL(1) .LE. ZERO .OR. XH(1) .GT. TWO) RETURN STAB 062
C     IF (XL(1) .GT. XB(2) .OR. XL(2) .GT. XB(2) .OR. XB(2) .GT. XH(2)) STAB 063
C     IF (XL(2) .LE. ZERO .OR. XH(2) .NE. ZERO) RETURN STAB 064
C     IF ((XL(2) .NE. ZERO) .AND. (XL(1) .LT. ONE .OR. XL(1) .GT. ONE)) STAB 065
C     IF ((XL(2) .NE. ZERO) .AND. (XL(1) .LT. ONE .AND. XH(1) .GT. ONE)) STAB 066
C     IF (XL(1) .GT. XB(3) .LE. ZERO) RETURN STAB 067
C     IF (ISCLBD .NE. 0 .AND. (XL(3) .GT. XB(3) .OR. XL(3) .GT. XH(3))) STAB 068
C     IF (XB(3) .GT. XH(3)) RETURN STAB 069
C     IF (ISCLBD .LT. 0 .AND. XL(3) .NE. XH(3)) RETURN STAB 070
C     IF (LOCBND .NE. 0 .AND. (XL(4) .GT. XB(4) .OR. XB(4) .GT. XH(4))) STAB 071
C     IF (XB(4) .GT. XH(4)) RETURN STAB 072
C     IF (LOCBND .LT. 0 .AND. XL(4) .NE. XH(4)) RETURN STAB 073
C     IF (LOCBND .NE. 0 .AND. XL(1) .EQ. ONE .AND. XH(1) .EQ. ONE) RETURN STAB 074
C     IF (LOCBND .LT. 0 .AND. XL(1) .NE. XH(1)) RETURN STAB 075
C     IF (LOCBND .NE. 0 .AND. XL(2) .EQ. ONE .AND. XH(2) .EQ. ONE) RETURN STAB 076
C     IF (LOCBND .LT. 0 .AND. XL(2) .NE. XH(2)) RETURN STAB 077
C     IF (LOCBND .NE. 0 .AND. XL(3) .EQ. ONE .AND. XH(3) .EQ. ONE) RETURN STAB 078
C     IF (LOCBND .LT. 0 .AND. XL(3) .NE. XH(3)) RETURN STAB 079
C     IF (LOCBND .NE. 0 .AND. XL(4) .EQ. ONE .AND. XH(4) .EQ. ONE) RETURN STAB 080
C     IF (LOCBND .LT. 0 .AND. XL(4) .NE. XH(4)) RETURN STAB 081
C     *XL(2) .NE. ZERO .OR. XL(2) .NE. XH(2)) RETURN STAB 082
C
C INITIAL ADJUSTMENT OF LOCATION/SCALE PARAMETERS/BOUNDS.
C
C SAVE BOUNDS FOR EXIT.
C
C WORK(NPAR + 5) = XL(3)
C WORK(NPAR + 6) = XH(3)
C WORK(NPAR + 7) = XL(4)
C WORK(NPAR + 8) = XH(4)
C XK = FLOAT(KSUM)
C
C LOCATION
C
C XKW = XK * XB(4)
C IF (LOCBND .LT. 0) GO TO 10
C IF (LOCBND .GT. 0) GO TO 20
C XL(4) = -FIVE
C XK(4) = FIVE
C GO TO 30
C
C 10 XL(4) = ZERO
C XH(4) = ZFRO
C GO TO 30
C
C 20 XL(4) = XK * XL(4)
C XK(4) = XK * XH(4)
C
C SCALE
C
C 30 XTOL = XK ** (ONE/XB(1))
C SIGMA = XTOL * XB(3)
C IF (ISCLBD .LT. 0) GO TO 40
C IF (ISCLBD .GT. 0) GO TO 50
C XL(3) = PT2
C XH(3) = FIVE
C GO TO 60
C
C 40 XL(3) = ONE
C XH(3) = ONE
C GO TO 60
C
C 50 XL(3) = XTOL * XL(3)
C XH(3) = XTOL * XH(3)
C
C EXPLICITLY SET XTOL TO E04KBF DEFAULT VALUE, USING X02AAF,
C SO THAT IT IS AVAILABLE ON EXIT ON E04KBF.
C 60 XTOL = TEN * SQRT(X02AAF(XTOL))
C

```

```

C      MEMORY MANAGEMENT
      MW = 2 * NPAR
      IWORK(MW + 2) = MODE
      IWORK(MW + 3) = IUNIT
      IWORK(MW + 4) = NPTS
      IWORK(MW + 5) = 9 * NPAR + 2
      LW = 6
      LW = LW - 8 - 2 * NPAR - LHESL
      MHESL = 9 * NPAR
      MHESD = MHESL + LHESL
      MN = MHESD + NPAR
      NPTS = MN + 9 * NPAR + 2
      MMT = NPTS + NPTS2
      MECF = MMT + NPTS
      MDERIV = MECF + NPTS
      AVOID UNCLEAR REFERENCES TO A AND A INVERSE IF MODE . NE. 0
      MA = MDERIV
      MAINV = MDERIV
      IA = NPTS + 1
      IF (MODE . NE. 0) GO TO 70
      MA = MA + (NPAR + 1) * NPTS
      MAINV = MA + IA * NPTS
      LOOPING POINT FOR ITERATION
      C 70 IWORK(1) = IWORK(1) + 1
      IDFLW = 0
      C  IF LOCATION/SCALE PARAMETERS ARE CONSTRAINED, UPDATE
      C  THEIR BOUNDS.
      C  IF (ISCLBD .LE. 0) GO TO 80
      XL(3) = AMIN(ONE,AMIN(FIVE,WORK(NPAR + 5)/SIGMA))
      XH(3) = AMAX(ONE,AMIN(FIVE,WORK(NPAR + 6)/SIGMA))
      80 IF (LOCBND .LE. 0) GO TO 90
      XL(4) = AMIN(ZERO,AMAX(FIVE,(WORK(NPAR + 7) - XMU)/SIGMA))
      XH(4) = AMAX(ZERO,AMIN(FIVE,(WORK(NPAR + 8) - XMU)/SIGMA))
      C  CHANGE PARAMETERS TO REFLECT FUTURE STANDARDIZATION.
      C  90 XB(3) = ONE
      XB(4) = ZERO
      WORK(NPAR + 3) = XB(1)
      WORK(NPAR + 4) = XB(2)
      SET INTYPE = 3 IF POSSIBLE, SO OLD HESSIAN CAN BE USED.
      C  INTYPE = 0
      IF (IWORK(1) .EQ. 1) GO TO 110
      INTYPE = 3
      DO 100 I = 1, NPAR
      IF (IWORK(I + 1) .GT. 0) GO TO 100
      INTYPE = 0
      GO TO 110
      100 CONTINUE
      C  SET GRIDPOINTS, WEIGHTS.
      C  110 CALL GRIDWT(XB, NPAR, XLM, TAU, WORK(NPTS), NPTS2, WORK(MMT),
      *NPTS, MODE, KSUM)
      C  SET E. CH. F. VALUES, ALSO A AND A INVERSE, IF MODE = 0, USING
      FIRST COL. OF DERIV AS WORKSPACE.
      CALL SETECFX, N, XB, NPAR, MODE, TAU, SIGMA, XMU, KSUM, IA,
      *NPTS2, NPTS, WORK(NPTS), WORK(MECF), WORK(MA), WORK(MAINV),
      *WORK(MDERIV), IFAULT)
      IF (IAULT .GT. 0) IFAULT = 9 + !FAULT
      IF (IAULT .EQ. 10 .OR. IFAULT .EQ. 11) GO TO 180
      C

```

```

C  CALL OR RESTART M.A.G. ROUTINE E04KBF
C  120 IF(AUTO = 1)
      CALL E04KBF(NPAR, FUNCT, MONIT, IPRINT, LOCSCN, INTYPE, E04LBS,
      *MAXCAL, ETA, XTOL, STEPMX, FEST, IBOUND, XL, XH, XB, WORK(MHESL),
      *LHESL, WORK(MHESD), IWORK(2), WORK(2), WORK(3), IWORK(MIW), LIW,
      *WORK(MW), LW, IFAULT)
      C   COMPUTE CONVERGENCE CRITERION
      WORK(1) = AMAX1(ABS(XB(3)) - ONE) ABS(XB(4))
      IF ((ISCBBD .LT. 0) AND. LOCBD .LT. 0) WORK(1) = AMAX1(ABS(XB(1)) -
      * WORK(NPAR + 3)) ABS(XB(2)) - WORK(NPAR + 4))
      C   OUTPUT IF REQUESTED
      IF (IUNIT .GT. 0) WRITE (IUNIT,1000) IWORK(1), IFAULT, WORK(1)
      IF (IAUTO .EQ. 0) GO TO 140
      IF (IAUTO .EQ. 1) GO TO 180
      IF (IAUTO .EQ. 12) GO TO 180
      IF (IAUTO .NE. 14) GO TO 130
      IF (IOVFLW .GE. 1) GO TO 180
      IOVFLW = IOVFLW + 1
      INTYPE = 0
      GO TO 120
      C   IF IFAULT = 113 OR 15, TEST PROJECTED GRADIENT AND PROJECTED
      C   MESSIAN CONDITION NUMBER
      130 IND = MN + 9 * NPAR
      IF (SQR10*NWORK(IND + 1) .LT. XTOL .AND. WORK(IND) .LT. ONE/WORK(
      *IND + 1)) IFAULT = 0
      C   UPDATE LOCATION AND SCALE AND TEST CONVERGENCE
      140 XMU = XMU + SIGMA * XB(4)
      IF (XB(1) .EQ. ONE) XMU = XMU + SIGMA * TWOVPI * XB(2) * XB(3) *
      *ALOG(XB(3))
      SIGMA = SIGMA * XB(3)
      IF (WORK(1) .LT. TOL) GO TO 150
      IF (IWORK(1) .LT. MAXIT) GO TO 70
      C   MAXIT ITNS HAVE BEEN USED WITHOUT CONVERGENCE - SET IFAULT.
      IND = 16
      IF (IAUTO .EQ. 13) IND = 17
      IF (IAUTO .EQ. 15) IND = 18
      IF (IAUTO = IND)
      C   TERMINATION WITH IFAULT = 0, 13, 15, 16, 17 OR 18
      150 IF (KSUM .GT. 1 .OR. ICOV .LT. 0) GO TO 190
      C   PREPARE TO CALL VARIAB TO COMPUTE COVARIANCE MATRICES.
      C   MEMORY MANAGEMENT.
      MHWORK = MDERIV + NPAR * NPTS
      MV = MN + NPAR * (NPAR + 1)
      C   REARRANGE THE M.A.G. ISTATE VECTOR SO IT HOLDS FREE
      C   PARAMETER SUBSCRIPTS IN INCREASING ORDER.
      NVAR = 0
      DO 160 I = 1, NPAR
      IF ((IWORK(I + 1) .LT. 0) .OR. (IWORK(I + 1) = 1))
      NVAR = NVAR + 1
      IWORK(NVAR + 1) = 1
      160 CONTINUE

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C IN THE RARE EVENT THAT THERE ARE NO FREE VARIABLES, VARIAB
C IS NOT CALLED AND COVARIANCE MATRICES ARE SET TO ZERO.
C IF (NVAR .GT. 0) GO TO 170
C IF (ICOV .EQ. 0) CALL FO1CAF(VCV1, NPAR, NPAR, IWORK(3))
C CALL FO1CAF(VCV2, NPAR, NPAR, IWORK(3))
C GO TO 190
C 170 NVARI = NVAR + 1
C XB(3) = ONE
C XB(4) = ZERO
C COMPUTE ESTIMATED ASYMPTOTIC COVARIANCE MATRICES.
C CALL VARIAB(ICOV, X, N, XB, NPAR, MODE, SIGMA, XMU, IWORK(2),
C *NVAR, WORK(NPTS), NPTS2, WORK(MHM1), WORK(MECF), NPIS,
C *WORK(MDERIV), WORK(MWORK), WORK(MHESD), WORK(MA), LA,
C *WORK(MAINV), VCV1, VCV2, WORK(MM), NVARI, WORK(MV), WORK(MW),
C *LW, WORK(MW), LW, IND, IND1)
C SAVE FAULT INDICATORS AND NO. OF ITNS TAKEN FOR HESSIAN.
C IWORK(2) = IND
C IWORK(3) = IND1
C IWORK(4) = IWORK(MW)
C GO TO 190
C EXIT FOR IFAULT = 10, 11, 12, OR 14, IF IFAULT = 12 OR 14,
C RESULTS OF THE LAST (ABORTED) OPTIMIZATION ARE NOT USED.
C 180 IWORK(2) = IFAULT
C IWORK(3) = IFAULT
C
C EXIT FOR IFAULT = 0, 13, 15, 16, 17, OR 18.
C RESET LOCATION SCALÉ BOUNDS
C 190 XL(3) = WORK(NPAR + 5)
C XH(3) = WORK(NPAR + 6)
C XL(4) = WORK(NPAR + 7)
C XH(4) = WORK(NPAR + 8)
C
C ADJUST PARAMETERS TO STANDARD FORM
C IF (XB(1) .EQ. ONE) XMU = XMU - TWOPI * XB(2) * SIGMA * ALOGI
C *SIGMA)
C XB(4) = XMU / XK
C XB(3) = SIGMA / (XK**(ONE/XB(1)))
C
C 1000 FORMAT (10H0MAJOR ITN, 13, 16H, IFAIL (E04KBF) =, I1, 3,
C *25H, CONVERGENCE CRITERION, =, E11.3)
C
C*****CALCULATES (POSITIVE) GRIDPOINTS AND ALL WEIGHTS.
C*****CALLED BY - STABLE
C*****CALLS - CHARN
C*****SUBROUTINE GRIDMT(PAR, NPAR, XLM, TAU, PTS, NPTS2, WT, NPTS,
C *MODE, KSUM)
C*****ARGUMENTS
C*****INTEGER IND, IND1, IND2, INNER
C*****REAL PAR(NPAR), XLM, TAU, PTS(NPTS2), WT(NPTS)
C*****LOCAL SCALARS
C*****LOGICAL FLAG
C*****INTEGER IND, IND1, IND2, INNER
C*****REAL ALPHA, AFAC1, AFAC2, TEMP, GAP, END, C1
C*****CONSTANTS
C*****REAL ZERO, PT025, PT035, PT045, PT055, PT065, PT075,
C *****PT075, PT3, PT5, PT6, PT8, PT9, ONE, ONEPI12, ONEPI16,

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*ONEPT7, ONEPT6, TWO, THREE, THRPT3, THRPT6, FOUR, FIVE, SEVEN, TENGRI 018
DATA ZERO, PT025, PT04, PT045, PT0425, PT05, PT06, PT07, GRID 019
*PT075, PT3, PT5, PT6, PT8, PT9, ONE, ONEPT2, ONEPT4, ONEPT6, GRID 020
*ONEPT7, ONEPT8, TWO, THREE, THRPT3, THRPT6, FOUR, FIVE, SEVEN, GRID 021
*TEN / 0.0, 0.025, 0.04, 0.0425, 0.045, 0.05, 0.06, 0.07, GRID 022
*0.075, 0.3, 0.5, 0.6, 0.8, 0.9, 1.0, 1.2, 1.4, 1.6, 1.7, 1.8, 2.0, GRID 023
*3.0, 3.3, 3.6, 4.0, 5.0, 7.0, 10.0, GRID 024
GRID 025
GRID 026
GRID 027
GRID 028
GRID 029
GRID 030
GRID 031
GRID 032
GRID 033
GRID 034
GRID 035
GRID 036
GRID 037
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GRID 039
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GRID 068
GRID 069
GRID 070
GRID 071
GRID 072
GRID 073
GRID 074
GRID 075
GRID 076
GRID 077

C
C   SELECT NUMBER OF INNER PTS = 2 IF NPTS .LT. 30, 3 IF NPTS .GE. 30.
C
C   INNER = 2
IF (NPTS .GE. 30) INNER = 3
ALPHA = PAR(1)
IF (ALPHA .LE. ONE) GO TO 70

C
C   CASE WHEN ALPHA .GT. 1 - FIRST CHOOSE RIGHT ENDPOINT.
C
END = THREE
IF (ALPHA .LT. ONEPT8) END = THRPT3
IF (ALPHA .LT. ONEPT7) END = THRPT6
IF (KSUM .EQ. 1) GO TO 20

C
C   WHEN KSUM = 1, EQUISPACE POINTS.
C
TEMP = ZERO
GAP = END / FLOAT(NPTS2)
DO 10 I = 1, NPTS2
TEMP = TEMP + GAP
PTS(I) = TEMP
10 CONTINUE
GO TO 100

C
C   WHEN KSUM .GT. 1 - FIRST USE HALF OF F-M ALPHA OPTIMAL CAPS
C
FOR POINTS CLOSE TO ORIGIN.
C
20 IF (NPTS .GE. 30) GO TO 30
GAP = PT075
IF (ALPHA .LT. ONEPT8) GAP = PT06
IF (ALPHA .LT. ONEPT6) GAP = PT07
IF (ALPHA .LT. ONEPT4) GAP = PT075
IF (ALPHA .LT. ONEPT2) GAP = PT0425
GO TO 40
30 GAP = PT05
IF (ALPHA .LT. ONEPT8) GAP = PT035
IF (ALPHA .LT. ONEPT6) GAP = PT04
IF (ALPHA .LT. ONEPT4) GAP = PT045
IF (ALPHA .LT. ONEPT2) GAP = PT025
40 TEMP = ZERO
DO 50 I = 1, INNER
TEMP = TEMP + GAP
PTS(I) = TEMP
50 CONTINUE

C
C   LOGARITHMICALLY SPACE THE REST OF THE POINTS BY LOG(1 + U / 2)
C
TEMP = ALOG(ONE + TEMP/TWO)
GAP = (ALOG(ONE + END/TWO) - TEMP) / FLOAT(NPTS2 - INNER)
IND = INNER +
DO 60 I = IND, NPTS2
TEMP = TEMP + GAP
PTS(I) = TWO * (EXP(TEMP) - ONE)
60 CONTINUE
GO TO 100
C

```

```

C CASE WHEN ALPHA .LE. 1 - SUBTRACT 1 FROM NO. OF INNER PTS
C IF ALPHA .LE. 1/2, START BY EQUISPACING ALL POINTS FOR
C LOC(U + (MAX(ALPHA, 0.3)**3) * 2 / 4, (THE LATTER MULTIPLICATION IS
C OMITTED IF KSUM .GT. 1.) THEN CONTINUE SPACING.
C 70 END = FIVE
C IF (ALPHA .LT. ONE) END = FOUR
C IF (AFAC1 = AFAC1 * AFAC1 * AFAC1) * FOUR
C IF (ALPHA .LT. PT9) END = FIVE
C IF (ALPHA .LT. PT0) END = SEVEN
C IF (ALPHA .LT. PT6) END = TEN
C AFAC1 = AMAX1(ALPHA, PT3)
C AFAC2 = ONE
C IF (KSUM .EQ. 1) AFAC2 = AFAC1 * AFAC1 / FOUR
C AFAC1 = AFAC1 * AFAC1 * AFAC1
C TEMP = ALOG(AFAC1)
C CI = ALOG(END + AFAC1)
C GAP = (CI - TEMP) / FLOAT(NPTS2)
C IF (ALPHA .LE. PT5) INNER = INNER - 1
C DO 80 I = 1, INNER
C TEMP = TEMP + GAP
C PTS(1) = (EXP(TEMP) - AFAC1) * AFAC2
C 80 CONTINUE
C TEMP = ALOG(PIS(INNER) + AFAC1)
C GAP = (CI - TEMP) / FLOOR(NPTS2 - INNER)
C IND = INNER + 1
C DO 90 I = IND, NPTS2
C TEMP = TEMP + GAP
C PTS(I) = EXP(TEMP) - AFAC1
C 90 CONTINUE
C
C COMPUTE WEIGHTS (ALL NPTS OF THEM).
C C IF KSUM .GT. 1, ALL WEIGHTS ARE 1.
C 100 IF (KSUM .EQ. 1) GO TO 120
C DO 110 I = 1, NPTS
C 110 WT(I) = ONE
C RETURN
C
C 120 FLAG = MODE .NE. 0
C IND = NPTS2 + 1
C DO 140 I = 1, NPTS2
C TEMP = PIS(1)
C IND1 = NPTS2 + 1
C IND2 = IND - 1
C GAP = EXP(-XIAM*TEMP**ALPHA)
C IF (FLAG) GO TO 130
C WT(IND1) = GAP
C WT(IND2) = GAP
C GO TO 140
C 130 GAP = GAP * GAP
C CALL CHARFN(TEMP, PAR, NPAR, END, AFAC1)
C CALL CHARFN(TEMP, + TEMP, PAR, NPAR, AFAC2, CI)
C WT(IND1) = GAP / (ONE + TAU*(CI - {END + AFAC1)**2))
C WT(IND2) = GAP / (ONE - TAU*(CI + {END - AFAC1)**2))
C 140 CONTINUE
C
C RETURN
C *****
C ***** COMPUTES REAL AND IMAGINARY PARTS OF STANDARD STABLE
C CHARACTERISTIC FUNCTION (SIGMA = 1, MU = 0).
C
C***** GRID 078
C***** GRID 079
C***** GRID 080
C***** GRID 081
C***** GRID 082
C***** GRID 083
C***** GRID 084
C***** GRID 085
C***** GRID 086
C***** GRID 087
C***** GRID 088
C***** GRID 089
C***** GRID 090
C***** GRID 091
C***** GRID 092
C***** GRID 093
C***** GRID 094
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C***** GRID 114
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C***** GRID 117
C***** GRID 118
C***** GRID 119
C***** GRID 120
C***** GRID 121
C***** GRID 122
C***** GRID 123
C***** GRID 124
C***** GRID 125
C***** GRID 126
C***** GRID 127
C***** GRID 128
C***** GRID 129
C***** GRID 130
C***** GRID 131
C***** GRID 132
C***** GRID 133
C***** GRID 134
C***** CHAR 001
C***** CHAR 002
C***** CHAR 003

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C ***** CALLED BY - GRIDWT, SETECF, VARIAB
C ***** SUBROUTINE CHARFN(U, PAR, NPAR, RE, XIM)
C   ARGUMENTS
C     INTEGER NPAR
C     REAL U, PAR(NPAR), RE, XIM
C   LOCAL SCALARS
C     REAL ALPHA, XMOD, ZERO, ONE, PIBY2
C     DATA ZERO, ONE, PIBY2 /0.0, 1.0, 1.570796327/
C
C     RE = ABS(U)
C     ALPHA = PAR(1)
C     IF (ALPHA .NE. ONE) GO TO 10
C     XIM = ZERO
C     IF (U .NE. ZERO) XIM = ALOG(RE) / PIBY2
C    GO TO 20
C 10  XIM = TAN(PIBY2*ALPHA)
C     XIM = -PAR(2) * SIGN(XMOD, U) * XIM
C 20  XMOD = RE ** ALPHA
C     XMOD = EXP(-XMOD)
C     RE = XMOD * COS(XIM)
C     XIM = XMOD * SIN(XIM)
C
C     RETURN
C
C***** FUNCTION/DERIVATIVE EVALUATION,
C***** CALLED BY - E04KBF, VARIAB, HESDIF
C***** SUBROUTINE FUNCT(IFLAG, N, XC, FC, GC, IW, LIW, W, LW)
C   ARGUMENTS
C     INTEGER IFLAG, N, LIW, IW(LIW), LW
C     REAL XC(N), FC, GC(N), W(LW)
C   LOCAL SCALARS
C     LOGICAL ALF1, LFLAG
C     INTEGER ILOW, IPTS, NPTS2, IND, IND1, ISUB, IPTS1, IW1,
C     *IECF, IDERIV, IPSI
C     REAL ALPHA, BSIGN, SIGMA, XMU, OMEGA, XMOD, PTS1, SINE, COSINE,
C     *PISSEC2, SUEXP, XLOGSU, FAC, Z, Z1, ZERO, ONE, PIBY2
C     DATA ZERO, ONE, PIBY2 /0.0, 1.0, 1.570796327/
C
C     ALPHA = XC(1)
C     BSIGN = XC(2)
C     SIGMA = XC(3)
C     XMU = XC(4)
C     ALF1 = ALPHA .EQ. ONE
C     LFLAG = IFLAG .EQ. 0
C
C   VARIABLES TO AID ADDRESSING IN W VECTOR - IPTS = ONE LESS THAN
C   POSITION OF FIRST POSITIVE GRIDPOINT IN W VECTOR, ETC.
C
C     NPTS = IW(5)
C     NPTS2 = NPTS / 2
C     IND = NPTS + 1
C     ILOW = NPTS2 + 1
C     IPTS = IW(6)
C     IW1 = IPTS + NPTS2
C     IECF = IW1 + NPTS
C     IDERIV = IECF + NPTS
C     IPS1 = IDERIV + N * NPTS
C     NPTS2 = IPTS - NPTS2

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C IF ALPHA .NE. 1, COMPUTE OMEGA(U,ALPHA) AND ITS DERIVATIVE W. R. FUNC 036
C TO ALPHA OUTSIDE MAIN LOOP. FUNC 037
C IF (ALF1) GO TO 10 FUNC 038
C OMEGA = TAN(PIBY2*ALPHA) FUNC 039
C PISEC2 = PIBY2 * (ONE + OMEGA*OMEGA) FUNC 040
C LOOP OVER POSITIVE GRID PTS (SCN(U) IGNORED), SAVE PSI AND FUNC 041
C ITS GRADIENT AT ALL GRID PTS (PSI(U) = RE(PHI(U)) + FUNC 042
C IM(PHI(U)) - EMPIRICAL COUNTERPARTS.) FUNC 043
C 10 DO 20 I = (LOW, NPTS) FUNC 044
C IMD1 = IMD - 1 FUNC 045
C ISUB = NPTS2 + 1 FUNC 046
C PSI1 = WI(ISUB) FUNC 047
C XLOGSU = SIGMA * PSI1 FUNC 048
C SUEXP = XLOGSU ** ALPHA FUNC 049
C XLOGSU = ALOG(XLOGSU) FUNC 050
C IF (ALF1) OMEGA = XLOGSU / PIBY2 FUNC 051
C COSINE = XMU * PSI1 - SUEXP * BSIGN * OMEGA FUNC 052
C SINE = SIN(COSINE) FUNC 053
C COSINE = COS(COSINE) FUNC 054
C XMOD = EXP(-SUEXP) FUNC 055
C SUEXP = SUEXP * XMOD FUNC 056
C
C SAVE COMPONENTS OF PSI FUNC 057
C ISUB = I PSI1 + 1 FUNC 058
C ISUB1 = IECF + 1 FUNC 059
C WI(ISUB) = XMOD * (COSINE + SINE) - WI(ISUB1) FUNC 060
C ISUB = I PSI1 + IMD1 FUNC 061
C ISUB1 = IECF + IMD1 FUNC 062
C WI(ISUB) = XMOD * (COSINE - SINE) - WI(ISUB1) FUNC 063
C IF (LFLAG) GO TO 20 FUNC 064
C
C CALCULATE DERIVATIVES IF REQUIRED FUNC 065
C
C DERIVATIVES W. R. TO ALPHA FUNC 066
C FAC = XLOGSU * OMEGA FUNC 067
C IF (.NOT. ALF1) FAC = FAC + PISEC2 FUNC 068
C FAC = FAC * BSIGN FUNC 069
C Z = FAC + XLOGSU FUNC 070
C Z1 = FAC - XLOGSU FUNC 071
C ISUB = IDERIV + 1 FUNC 072
C WI(ISUB) = SUEXP * (-Z*COSINE + Z1*SINE) FUNC 073
C ISUB1 = IDERIV + IMD1 FUNC 074
C WI(ISUB1) = SUEXP * (Z1*COSINE + Z*SINE) FUNC 075
C
C DERIVATIVES W. R. TO BETA FUNC 076
C FAC = SUEXP * OMEGA FUNC 077
C ISUB = ISUB + NPTS FUNC 078
C WI(ISUB) = FAC * (SINE - COSINE) FUNC 079
C ISUB1 = ISUB1 + NPTS FUNC 080
C WI(ISUB1) = FAC * (SINE + COSINE) FUNC 081
C
C DERIVATIVES W. R. TO SIGMA FUNC 082
C FAC = BSIGN * OMEGA FUNC 083
C Z = ONE + FAC FUNC 084
C Z1 = ONE - FAC FUNC 085
C FAC = -ALPHA * SUEXP / SIGMA FUNC 086
C ISUB = ISUB + NPTS FUNC 087
C WI(ISUB) = FAC * (Z*COSINE + Z1*SINE) FUNC 088
C ISUB1 = ISUB1 + NPTS FUNC 089

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      W(IISUB1) = FAC * (Z1*COSINE - Z2*SINE)
C   C   DERIVATIVES W. R. TO MU
      FAC = PTSI * XMOD
      ISUB = ISUB + NPTS
      W(IISUB) = FAC * (-SINE + COSINE)
      ISUB1 = ISUB1 + NPTS
      W(IISUB1) = -FAC * (SINE + COSINE)
      20 CONTINUE

C   C   NOW COMPUTE OBJECTIVE FUNCTION , OPTIONAL GRADIENT.
      FC = ZERO
      IF (LFLAG) GO TO 40
      ILOW = IDERIV - NPTS
      DO 30 I = 1, N
      30 GC(I) = ZERO
      40 IF (IM(3).EQ. 0) GO TO 70

C   C   SUM-OF-SQUARES ESTIMATION
      DO 60 I = 1, NPTS
      C   FN, EVALUATION
      ISUB = IPSI + I
      Z = W(IISUB)
      ISUB = INT + I
      Z1 = Z * W(IISUB)
      FC = FC + Z * Z1
      IF (LFLAG) GO TO 60
      C   GRADIENT EVALUATION IF REQUESTED.
      ISUB = ILOW + I
      Z1 = Z1 + Z1
      DO 50 J = 1, N
      ISUB = ISUB + NPTS
      GC(J) = GC(J) + W(IISUB) * Z1
      50 CONTINUE
      60 CONTINUE
      RETURN

C   C   MATRIX ESTIMATION - FIRST MULTIPLY PSI VALUES BY WEIGHTS.
      70 DO 80 I = 1, NPTS
      ISUB = IPSI + I
      ISUB1 = INT + I
      W(IISUB) = W(IISUB) * W(IISUB1)
      80 CONTINUE
      C   POSITION OF A INVERSE IS REQUIRED.
      IND1 = IPSI + IND * NPTS
      DO 110 I = 1, NPTS
      Z = ZERO
      IND1 = IND1 + NPTS
      C   SUM OVER J OF PSI(J) * AINV(I,J)
      DO 90 J = 1, NPTS
      ISUB := IPSI + J
      ISUB1 = IND1 + J
      Z = Z + W(IISUB) * W(IISUB1)
      90 CONTINUE
      C   MULTIPLY BY PSI(I) AND ADD TO FN. VALUE
      ISUB = IPSI + I
      FC = FC + Z * W(IISUB)
      IF (LFLAG) GO TO 110
      C   GRADIENT IF REQUESTED - FOR JTH COMPONENT OF GRADIENT ADD

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C      2*(JTH DERIVATIVE AT GRIDPOINT I)*WT(I)*(RESULT OF DO 90 LOOP) FUNC 156
C      ISUB = IWT + 1 FUNC 157
C      Z = (Z + Z) * W(I SUB) FUNC 158
C      ISUB = ILow + 1 FUNC 159
C      DO 100 J = 1, N FUNC 160
C      ISUB = ISUB + NPTS FUNC 161
C      GCI(J) = GCI(J) + Z * W(I SUB) FUNC 162
C      100 CONTINUE FUNC 163
C      110 CONTINUE FUNC 164
C
C      RETURN FUNC 165
C      END FUNC 166
C
C***** COMPUTES EMPIRICAL CH. F. VALUES, ADJUSTING FOR LOCATION,
C***** SCALE, AND K-SUM INDEX. FOR MATRIX ESTIMATION, THE UPPER
C***** TRIANGLE OF A MATRIX IS CALCULATED AND INVERTED.
C***** CALLED BY - STABLE
C***** CALLS - CHARFN
C***** SUBROUTINE SETEC(X, N, PAR, NPAR, MODE, TAU, SIGMA, XMU, KSUM,
C***** FO1ABF (ACCURATE INVERSION OF POSITIVE DEFINITE
C***** SYMMETRIC MATRIX).
C***** SUBROUTINE SETEC(X, N, PAR, NPAR, MODE, TAU, SIGMA, XMU, KSUM,
C***** "IA, NPTS2, NPTS, PTS, ECF, A, AINV, WORK, IFAULT)
C***** ARGUMENTS
C      INTEGER N, NPAR, MODE, KSUM, IA, NPTS2, NPTS, IFAULT
C      REAL X(N), PAR(NPAR), TAU, SIGMA, XMU, PTS(NPTS2), ECF(NPTS),
C      A(IA,NPTS), AINV(NPTS), WORK(NPTS)
C      LOCAL SCALARS
C      INTEGER IND, IND1, IND2, IND3
C      REAL PTSJ, RE, XIM, RE1, XIM1, RPI1, RPI1, RMI1, ZERO,
C      HALF
C      DATA ZERO, HALF /0.0, 0.5/
C
C      CALCULATION OF E.CH.F. VALUES
C      PTSJ = FLOAT(N)
C      XIM1 = FLOAT(KSUM)
C      RPI = XIM1 * HALF
C      IND = NPTS2 + 1
C      IND1 = NPTS + 1
C      DO 20 I = IND, NPTS
C      IND2 = I - NPTS2
C      PTSI = PTS(IND2) / SIGMA
C      IND2 = IND1 - I
C      RE = ZERO
C      XIM = ZERO
C
C      DO 10 J = 1, N
C      RPI1 = X(J) * PTSI
C      RE = RE + COS(RPI1)
C      XIM = XIM + SIN(RPI1)
C      10 CONTINUE
C
C      RE = RE / PTSJ
C      XIM = XIM / PTSJ
C      RMI = (RE*RE + XIM*XIM)**0.5
C      RPI1 = XIM * ATAN2(XIM, RE) - XMU + PTSI
C      RE = RMI * COS(RPI1)
C      XIM = RMI * SIN(RPI1)
C      ECF(I) = RE + XIM

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      ECF(IND2) = RE - XIM
      20 CONTINUE
C     SET UPPER TRIANGLE OF A IF REQUESTED. A GENERATED FROM
C     POSITIVE GRIDPOINTS ONLY - ANTI DIAGONAL COMPUTED TWICE.
C     IF (MODE .NE. 0) RETURN
C     FIRST FILL WORK WITH (RE + IM) (PHI) TO SAVE EVALS.
      DO 30 I = IND, NPTS
      IND2 = I - NPTS2
      CALL CHARFM(PTS(IND2), PAR, NPAR, RE, XIM)
      IND2 = IND1 - 1
      WORK(1) = RE + XIM
      WORK(IND2) = RE - XIM
      30 CONTINUE
C     COMPUTATION OF A.
      DO 40 I = IND, NPTS
      IND2 = I - NPTS2
      PTS1 = PTS(IND2)
      IND2 = IND1 - 1
      RP1 = WORK(1)
      RM1 = WORK(IND2)
      DO 40 J = IND, 1
      IND3 = J - NPTS2
      PTSJ = PTS(IND3)
      IND3 = IND1 - J
      RP1 = WORK(J)
      RM1 = WORK(IND3)
      CALL CHARFN(PTS1 + PTSJ, PAR, NPAR, RE, XIM)
      CALL CHARFN(PTS1 - PTSJ, PAR, NPAR, RE, XIM)
      AI(J,1) = RE1 + XIM - RP1 * RP1
      AI(IND2,J) = RE - XIM1 - RM1 * RP1
      AI(IND3,1) = RE + XIM - RP1 * RM1
      AI(IND2,IND3) = RE1 - XIM - RM1 * RM11
      40 CONTINUE
C     DIAGONAL OF A ADDITIVELY INFLATED BY TAU TIMES AVERAGE OF
C     DIAGONAL ELEMENTS.
      IF (TAU .EQ. ZERO) GO TO 70
      PTS1 = ZERO
      DO 50 I = 1, NPTS
      PTS1 = PTS1 + AI(I,1)
      PTS1 = TAU * PTS1 / FLOAT(NPTS)
      DO 60 I = 1, NPTS
      AI(I,1) = AI(I,1) + PTS1
      60 AI(I,1) = A(I,1) + PTS1
      70 IAULT = 1
      CALL FO1ABF(A, IA, NPTS, AINV, NPTS, WORK, IAULT)
      C     EXIT IF A FOUND NON POSITIVE DEFINITE OR ILL-CONDITIONED.
      IF (IAULT .GT. 0) RETURN
      C     ARRANGE A INVERSE SO IT IS COMPLETELY FILLED.
      DO 80 I = 1, NPTS
      DO 80 J = 1, I
      AINV(J,I) = AINV(I,J)
      80 CONTINUE
      C     INVERT A USING N.A.G. ROUTINE FO1ABF
      C     IAULT = 1
      CALL FO1ABF(A, IA, NPTS, AINV, NPTS, WORK, IAULT)
      C     EXIT IF A FOUND NON POSITIVE DEFINITE OR ILL-CONDITIONED.
      IF (IAULT .GT. 0) RETURN
      C     ARRANGE A INVERSE SO IT IS COMPLETELY FILLED.
      DO 90 I = 1, NPTS
      DO 90 J = 1, I
      AINV(J,I) = AINV(I,J)
      90 AINV(I,J) = AINV(I,J)
      80 CONTINUE
      C     RETURN
      END
C     *****MONITORING OF E04KBF.
      C     MON1 001
      C     MON1 002

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C CALLED BY - E04KBF
C **** SUBROUTINE MONIT(N, XC, FC, GC, ISTATE, GPJNRM, COND, POSDEF,
C *NITER, NF, LIW, LW, LM)
C LOGICAL POSDEF
C INTEGER N, ISTATE(N), NITER, NF, LIW, IW(LIW), LW
C REAL XC(N), FC, GC(N), GPJNRM, COND, WI(LW)
C LOCAL SCALAR
C INTEGER IUNIT
C
C STORE HESIAN CONDITION NUMBER AND PROJECTED GRADIENT NORM IN
C WORK VECTOR
IUNIT = 9 * N + 1
WI(IUNIT) = COND
WI(IUNIT + 1) = GPJNRM
IUNIT = IW(6)
IF (IUNIT .LE. 0) RETURN
C
C WRITE DETAILS OF OPTIMIZATION PROCESS IF IUNIT .GT. 0
WRITE (IUNIT,10) NITER, NF, FC, GPJNRM
WRITE (IUNIT,20) (XC(I), I=1,N)
WRITE (IUNIT,30) (GC(I), I=1,N)
WRITE (IUNIT,40) COND
C
C 10 FORMAT (SH01NS, 5X, SHFN EVALS, 8X, SHFN VALUE, 5X,
C *21HNORM OF PROJ GRADIENT/1H 16, 8X, 15, 5X, E11.4, 15X, E11.4)
20 FORMAT (10HSOLUTIONS, 4E13.5)
30 FORMAT (10H PROJ GRAD, 4E13.5)
40 FORMAT (5OH ESTIMATED CONDITION NUMBER OF PROJECTED HESSIAN = ,
C *E12.2)
RETURN
END
C
C CALCULATES EMPIRICAL (VCV1) AND ASYMPTOTIC (VCV2)
C APPROXIMATIONS TO ASYMMPTOTIC COVARIANCE MATRICES. IFAIL1 AND
C IFAIL2 ARE FAILURE INDICATORS FOR MATRIX INVERSION REQUIRED
C FOR VCV1, VCV2 RESPECTIVELY.
C CALLED BY - STABLE
C CALLS - HESDEF FUNCT, CHARFN, SETVCV, VMATRIX, DAPROD, HVPROD
C N.A.G. SUBROUTINES CALLED -
C FO1CAF (SETS A MATRIX TO ZERO),
C FO1CMF (SET ONE MATRIX TO ANOTHER).
C
C **** SUBROUTINE VARIAB(ICOV, X, N, PAR, MODE, SIGMA, XMU, ISUB,
C *NVAR, PTS, MPTS2, WI, ECF, NPTS, DERIV, WORK, HOLD, A, AINV,
C *VCV1, VCV2, H, NVAR, V, IW, LIW, LW, IFAIL2)
C ARGUMENTS
C INTEGER ICOV, N, NVAR, MODE, NVAR, I SUB(NVAR), NPTS2, NPTS, IA,
C *NVAR1, LIW, IW(LIW), LW, IFAIL1, IFAIL2
C REAL X(N), PAR(NPAR), SIGMA, XMU, PTS(NPTS2), WI(NPTS), ECF(NPTS),
C *DERIV(NPTS, NPAR), WORK(NPTS), HOLD(NVAR), A(NPTS),
C *AINV(NPTS, NPTS), VCV1(NPAR, NPAR), VCV2(NPAR, NPAR), H(NVAR1, NVAR),
C *V(NVAR, NVAR) WI(LW)
C LOCAL SCALARS
C LOGICAL FLAG
C INTEGER IND, IND1, IND2, IND3
C REAL PTSK, PTSL, RP1, RPI1, RPI11, RMI1, COVKL, COVM1, COVMK, COVM,
C *D1, D2, D3, D4, ZERO
C DATA ZERO /0.0/

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C      IND = NPTS2 + 1
C      IND1 = NPTS + 1
C
C      IF REQUESTED, FIRST CALCULATE HESSIAN FOR EMPIRICAL VERSION
C      AND STORE IN VCV1. (HESDIF FUNCT REQUIRE ECF, WORK,
C      POSSIBLY AINV, WHICH ARE USED AS WORK AREAS BELOW.)
C      H AND V ARE PASSED AS WORKSPACE.
C      IF (ICOV .EQ. 0) CALL HESDIF(PAR, NPAR, ISUB, VCV1, H, V, NVAR,
C      *IW, LIW, W, LW)
C
C      CALL FUNCT TO SET DERIV, AS GRID SEARCH PERFORMED BY E04KBF
C      MAY HAVE SET IT TO STRANGE VALUES. VCV2 USED AS WORKSPACE.
C      CALL FUNCT(2, NPAR, PAR, D1, VCV2(1,1), IW, LIW, W, LW)
C
C      SHIFT DERIV VALUES SO THEY CAN BE ADDRESSED WITHOUT THE
C      ISUB VECTOR. NOTE ISUB ELEMENTS ARE IN ASCENDING ORDER.
C
C      DO 20 I = 1, NVAR
C      IND2 = ISUB(I)
C      IF (IND2 .EQ. 1) GO TO 20
C      DO 10 J = 1, NPTS
C      10 DERIV(J, I) = DERIV(I, IND2)
C      20 CONTINUE
C
C      C
C      C      FILL ECF VECTOR WITH CH. F. VALUES, NOW THAT IT IS NO
C      C      LONGER NEEDED FOR FUNCTION EVALUATION.
C      DO 30 I = IND, NPTS
C      IND2 = I - NPTS2
C      CALL CHARFN(PTS(IND2), PAR, NPAR, D1, D2)
C      IND2 = IND1 - I
C      ECF(I) = D1 + D2
C      ECF(IND2) = D1 - D2
C      30 CONTINUE
C      IF (MODE .EQ. 0) GO TO 100
C
C      SUM OF SQUARES ESTIMATION SECTION.
C
C      FIRST DO ASYMPTOTIC VERSION.
C      CALCULATE UPPER TRIANGLE OF HESSIAN.
C      DO 50 I = 1, NVAR
C      DO 50 J = 1, NVAR
C      D1 = ZERO
C      40 K = 1, NPTS
C      D1 = D1 + DERIV(K, I) * DERIV(K, J) * WT(K)
C      H(I,J) = D1
C      50 CONTINUE
C
C      PREMULTIPLY DERIV BY WEIGHTS TO SAVE MULTIPLICATIONS.
C      DO 60 I = 1, NPTS
C      D1 = WT(I)
C      DO 60 J = 1, NVAR
C      DERIV(I,J) = D1 * DERIV(I,J)
C      60 CONTINUE
C
C      COMPUTE UPPER TRIANGLE OF V.
C      CALCULATING THE A MATRIX FOR MATRIX ESTIMATION, BUT
C      COMPLICATIONS ARISE IN COMPUTING BILINEAR FORMS.
C      CALL FD1CAFY, NVAR, NVAR, 1FAIL2)
C      DO 90 K = IND, NPTS
C      IND2 = K - NPTS2

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PTS1 = PTS(IND2)
IND2 = IND1 - K
RPI1 = ECF(K)
RMI1 = ECF(IND2)
DO 90 L = IND, K
IND3 = L - NP1S2
PTS1 = PTS(IND3)
IND3 = IND1 - L
RPI1 = ECF(L)
RM11 = ECF(IND3)
CALL CHARFN(PTS1 + PTS1, PAR, NPAR, D1, D2)
CALL CHARFN(PTS1 - PTS1, PAR, NPAR, D3, D4)
COVNL = D3 + D2 - RPI1 * RPI1
COVNL = D1 - D4 - RMI1 * RPI1
COVNL = D1 + D4 - RPI1 * RMI1
COVNL = D3 - D2 - RMI1 * RM11
FLAG = K .EQ. L
C      LOOP TO ADD CONTRIBUTIONS TO V (BILINEAR FORMS).
DO 80 I = 1, NVAR
D1 = DERIV(K, I)
D2 = DERIV(IND2, I)
DO 80 J = 1, NVAR
D3 = DERIV(L, J)
D4 = DERIV(IND3, J)
PTS1 = (COVNL*D1 + COVNL*D2) * D3 + (COVKM*D1 + COVM*D2) * D4
IF (FLAG) GO TO 70
C      WHEN K .NE. L, MUST ADD SYMMETRIC CONTRIBUTION.
RPI1 = DERIV(K, J)
RM11 = DERIV(IND2, J)
D3 = DERIV(L, I)
D4 = DERIV(IND3, I)
PTS1 = PTS1 + (COVKL*RPI1 + COVNL*RM11) * D3 + (COVKM*RP11 +
*COVM*RM11) * D4
70 V(I,J) = V(I,J) + PTS1
80 CONTINUE
90 CONTINUE
GO TO 140
C      MATRIX ESTIMATION SECTION.
C      FILL A MATRIX COMPLETELY (UPPER TRIANGLE ONLY ON ENTRY),
C      MULTIPLY ELEMENTS OF A BY CORRESPONDING WEIGHTS, MULTIPLY
C      DERIV VALUES BY WEIGHTS TO SAVE MULTIPLICATIONS LATER.
100 DO 130 I = 1, NP1S
D1 = WT(I)
DO 110 J = 1, NP1S
A(I,J) = A(I,J) * D1 * WT(J)
A(J,I) = A(I,J)
110 CONTINUE
DO 120 J = 1, NVAR
120 DERIV(I,J) = DERIV(I,J) * D1
130 CONTINUE
C      ASYMPTOTIC VERSION.
C      MULTIPLY AINV * DERIV, OVERWRITING CORNER OF AINV AND USING
C      HOLD AS WORKSPACE
C      CALL DAPROD(AINV, NP1S, NPTS, DERIV, HOLD, NVAR)
C      MULTIPLY A * (AINV CORNER), OVERWRITING CORNER OF A AND

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DO 50 I = 1, N
D1 = (X(I) - XMU) / SIGMA
C WORK HOLDS VECTOR OF SINE/COSINE TERMS.
DO 10 J = IND,NPTS
IND2 = J - NPTS*S2
D2 = PIS(IND2)* D1
D3 = COS(D2)
D2 = SIN(D2)
IND2 = IND1 - J
WORK(J) = ECF(J) - D3 - D2
WORK(IND2) = ECF(IND2) - D3 + D2
IF (FLAG) GO TO 10
C IF MATRIX ESTIMATION, MULTIPLY ELEMENTS OF WORK BY WEIGHTS.
C WORK(J) = WORK(J) * WT(J)
C WORK(IND2) = WORK(IND2) * WT(IND2)
10 CONTINUE

C MULTIPLY DERIV * WORK, WRITING RESULT TO HOLD. MULTIPLICATION
C DONE DIRECTLY TO AVOID OVERHEAD OF SUBROUTINE CALL.
DO 30 J = 1, NVAR
D1 = ZERO
DO 20 K = 1, NPTS
D2 = D1 + DERIV(K,J) * WORK(K)
HOLD(J) = D1
30 CONTINUE

C ADD HOLD * (HOLD TRANSPOSE) TO V.
DO 40 J = 1, NVAR
D1 = HOLD(J)
DO 40 K = J, NVAR
V(J,K) = V(J,K) + D1 * HOLD(K)
40 CONTINUE
50 CONTINUE

C FINAL CONSTANT FACTOR FOR V.
D1 = FOUR / FLOAT(N)
DO 60 I = 1, NVAR
DO 60 J = I, NVAR
60 V(I,J) = V(I,J) * D1
50 CONTINUE

C RETURN
END
C*****MULTIPLIES THE (NPTS BY NPTS) CORNER OF THE ((1 FAC1 BY NPTS)
C MATRIX FAC1 BY THE (NPTS BY NVAR) MATRIX FAC2, OVERWRITING
C THE UPPER LEFT (NPTS BY NVAR) ELEMENTS OF FAC1. UNFORTUNATELY,
C LOCAL SCALARS FAC1 AND FAC2 ARE NOT ALLOW THIS
C ROUTINE FOICKF DOES NOT ALLOW THIS
C KIND OF OVERWRITING.
C CALLED BY - VARIAB
C*****SUBROUTINE DAPR(DAPR(FAC1, 1FAC1, NPTS, FAC2, WORK, NVAR)
C ARGUMENTS
C INTEGER 1FAC1, NPTS, NVAR
C REAL FAC1((1FAC1, NPTS), FAC2(NPTS, NVAR), WORK(NVAR))
C LOCAL SCALARS
C REAL TEMP, ZERO
C DATA ZERO /0.0/

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C USING HOLD AS WORKSPACE.
C CALL DAPROD(A, IA, NPTS, AINV, HOLD, NVAR)
C
C MULTIPLY (A CORNER TRANSPOSE) * (AINV CORNER), GIVING
C UPPER TRIANGLE OF V.
C CALL HVPROD(A, IA, NVAR, AINV, NPTS, V, NVAR)
C
C MULTIPLY (AINV CORNER TRANSPOSE) * DERIV, GIVING UPPER
C TRIANGLE OF HESSIAN.
C CALL HVPROD(AINV, NPTS, NVAR, DERIV, NPTS, H, NVAR1)
C
C CODE COMMON TO MATRIX AND SUM OF SQUARES ESTIMATION.
C COMPUTE ASYMPTOTIC COVARIANCE MATRIX.
C 140 CALL SETVCV1(I SUB, NVAR, H, NVAR1, V, HOLD, VCV2, NPAR, SIGMA,
C *FAIL2)
C IF (ICOV .GT. 0) RETURN
C
C EMPIRICAL VERSION IF REQUESTED.
C COMPUTE EMPIRICAL V MATRIX, USING WORK AND HOLD AS WORK AREAS.
C IF (MODE .NE. 0) CALL VMATRIX(X, N, MODE, XNU, SIGMA, PTS, NPTS2,
C *WT, ECF, WORK, NPTS, DERIV, V, HOLD, NVAR)
C IF (MODE .EQ. 0) CALL VMATRIX(X, N, MODE, XNU, SIGMA, PTS, NPTS2,
C *WT, ECF, WORK, NPTS, AINV, V, HOLD, NVAR)
C
C RESTORE HESSIAN FROM VCV1, COMPUTE COVARIANCE MATRIX.
C CALL FO1CHF(VCV1, NVAR, H, NVAR1, NVAR, NVAR)
C CALL SETVCV1(I SUB, NVAR, H, NVAR1, V, HOLD, VCV1, NPAR, SIGMA,
C *FAIL1)
C
C RETURN
C END
C*****VHAT 001
C*****VHAT 002
C*****VHAT 003
C*****VHAT 004
C*****VHAT 005
C*****VHAT 006
C*****VHAT 007
C*****VHAT 008
C*****VHAT 009
C*****VHAT 010
C*****VHAT 011
C*****VHAT 012
C*****VHAT 013
C*****VHAT 014
C*****VHAT 015
C*****VHAT 016
C*****VHAT 017
C*****VHAT 018
C*****VHAT 019
C*****VHAT 020
C*****VHAT 021
C*****VHAT 022
C*****VHAT 023
C*****VHAT 024
C*****VHAT 025
C*****VHAT 026
C*****VHAT 027
C*****VHAT 028
C*****VHAT 029
C
C SUBROUTINE VMATRIX(X, N, MODE, XNU, SIGMA, PTS, NPTS2, WT, ECF,
C *WORK, NPTS, DERIV, V, HOLD, NVAR)
C ARGUMENTS
C INTEGER N, MODE, NPTS2, NPTS, NVAR
C REAL X(N), XNU, SIGMA, PTS, NPTS2, WT(NPTS), ECF(NPTS),
C *WORK(NPTS), DERIV(NPTS, NVAR), V(NVAR, NVAR), HOLD(NVVAR)
C LOCAL SCALARS
C LOGICAL FLAG
C INTEGER IND, IND1, IND2
C REAL D1, D2, D3, ZERO, FOUR
C DATA ZERO, FOUR /0.0, 4.0/
C
C SET V TO 0.
C FLAG = MODE .ME. 0
C IND = NPTS2 + 1
C IND1 = NPTS + 1
C CALL FO1CAF(V, NVAR, NVAR, IND2)
C
C MAIN LOOP OVER SAMPLE.

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DO 40 I = 1, NPTS
DO 20 J = 1, NVAR
TEMP = ZERO
DO 10 K = 1, NPTS
10 TEMP = TEMP + FAC1(I,K) * FAC2(K,J)
WORK(J) = TEMP
20 CONTINUE
DO 30 J = 1, NVAR
30 FAC1(I,J) = WORK(J)
40 CONTINUE
C
C      RETURN
END
C*****MULTIPLIES THE TRANPOSED (NPTS BY NVAR) CORNER OF THE
C      (IFAC1 BY NVAR) MATRIX FAC1 BY THE (NPTS BY NVAR) MATRIX
C      FAC2, GIVING THE UPPER TRIANGLE OF EITHER V OR H.
C*****CALLED BY - VARIAB
C*****SUBROUTINE HVPROD(FAC1, IFAC1, NVAR, FAC2, NPTS, VH, IVH)
C      ARGUMENTS
C      INTEGER IFAC1, NVAR, NPTS, IVH
C      REAL FAC1(IFAC1,NVAR), FAC2(NPTS,NVAR), VH(IVH,NVAR)
C      LOCAL SCALARS
C      REAL TEMP, ZERO
C      DATA ZERO /0.0/
C
C      DO 20 I = 1, NVAR
C      DO 20 J = 1, NVAR
TEMP = ZERO
DO 10 K = 1, NPTS
10 TEMP = TEMP + FAC1(K,I) * FAC2(K,J)
VH(I,J) = TEMP
20 CONTINUE
C
C      RETURN
END
C*****COMMON OPERATIONS IN COMPUTATION OF COVARIANCE MATRICES.
C      INVERTS HESIAN MATRIX H, CALCULATES (H INVERSE) * V *
C      (H INVERSE), OVERRWITTING V.
C*****CALLED BY - VARIAB
C      N.A.G. SUBROUTINES CALLED -
C          F01ABF (ACCURATE INVERSION OF POSITIVE DEFINITE
C          SYMMETRIC MATRIX),
C          F01CKF (MATRIX MULTIPLICATION WITH OVERWRITING),
C          F01CMF (SET ONE MATRIX EQUAL TO ANOTHER),
C          F01CAF (SET A MATRIX TO ZERO).
C*****SUBROUTINE SETVCV(I SUB, NVAR, H, NVARI, V, WORK, VCV, NPAR, SIGMA,
*FAULT)
C      ARGUMENTS
C      INTEGER NVAR, I SUB(NVAR), NVAR1, NPAR, IFAULT
REAL H(NVAR), NVAR, V(NVAR), WORK(NVAR), VCV(NPAR, NPAR),
*SIGMA
C      LOCAL SCALARS
C      INTEGER IND, IND1
REAL TEMP, ZERO
DATA ZERO /0.0/

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C      INVERT H, USING VCV AS WORKSPACE.
C
C      IFault = 1
C      CALL FO1ABF(H, NVAR1, NVAR, VCV, NPAR, WORK, IFAULT)
C      IF (IFault .EQ. 0) GO TO 10
C      ON FAILURE OF INVERSION, SET VCV TO 0 AND RETURN.
C      CALL FO1CAF(VCV, NPAR, NPAR, IND)
C      RETURN
C      FILL OUT VCV AND V (CURRENTLY ONLY HALF FULL).
C
C      10 DO 20 I = 1, NVAR
C      DO 20 J = 1, 1
C          V(I,J) = V(J,I)
C          VCV(I,J) = VCV(I,J)
C 20 CONTINUE
C
C      SET H TO ITS INVERSE IN SUCH A WAY THAT MULTIPLICATION VIA
C      FO1CMF WILL BE CORRECT. (NOTE DIMENSIONS IN FO1CMF CALL)
C      CALL FO1CMF(VCV, NPAR, H, NVAR, NVAR)
C
C      MULTIPLY H * V, OVERWRITING V.
C      CALL FO1CKF(V, H, V, NVAR, NVAR, WORK, NVAR, 3, IFAULT)
C
C      MULTIPLY V * H, OVERWRITING V.
C      CALL FO1CKF(V, V, H, NVAR, NVAR, WORK, NVAR, 2, IFAULT)
C
C      V NOW CONTAINS COVARIANCE MATRIX FOR FREE VARIABLES. ARRANGE
C      ITS CONTENTS IN VCV, ADJUST SIGMA AND MU ENTRIES FOR SCALE.
C      CALL FO1CAF(VCV, NPAR, NPAR, IFAULT)
C      DO 30 I = 1, NVAR
C      DO 30 J = 1, 1
C          IND = MIN0(I,SUB(1,1),SUB(J))
C          IND1 = MAX0(I,SUB(1,1),SUB(J))
C          VCV(IND,IND1) = V(I,J)
C 30 CONTINUE
C      DO 40 I = 1, NPAR
C      DO 40 J = 1, J
C          TEMP = SIGMA * VCV(I,J)
C          IF (I .GE. 3) TEMP = SIGMA * TEMP
C          VCV(I,J) = TEMP
C 40 CONTINUE
C
C      FILL LOWER TRIANGLE OF VCV WITH CORRELATIONS.
C      DO 50 I = 2, NPAR
C          TEMP = VCV(I,1)
C          IND = 1 - 1
C          DO 50 J = 1, IND
C              IF (AMIN1(TEMP, VCV(J,1)) .LE. ZERO) GO TO 50
C              VCV(I,J) = VCV(J,1) / SQRT(TEMP*VCV(J,J))
C 50 CONTINUE
C
C      RETURN
C      END
C*****HESD 001*****
C      COMPUTES APPROXIMATE UPPER TRIANGLE OF HESSIAN BY DIFFERENCES. HESD 002
C      NOTE THAT WITH IFLAG = 0, FUNCT WILL NOT SET A GRADIENT. HESD 003
C      CALLED BY - VARIAB HESD 004
C      CALLS - FUNCT HESD 005
C*****HESD 006*****
C      SUBROUTINE HESDIF(PAR, NPAR, ISUB, H, SAVE1, SAVE2, NVAR, IW, LIW, HESD 007
C      *W, LM) HESD 008
C      ARGUMENTS HESD 009

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      INTEGER NPAR, NVAR, ISUB(NVAR), LIW, IW(LIW), LW
      REAL PAR(NPAR), H(NVAR,NVAR), SAVE1(NVAR,NVAR), SAVE2(NVAR,NVAR),
     *W(LW)
      LOCAL SCALARS
      INTEGER ITER, IND, IND1, IND2, IND3
      REAL PARJ, TEMP, TEMP1, STEP, DENOM, ZERO, TOL, TENVN,
      *STEP1, ONE, TWO, SQRT10, FOUR
      DATA ZERO, TOL, TENVN, STEP1, ONE, TWO, SQRT10, FOUR / 0.0, 1.0E-6, HE SD 017
      *1.0E-4, 3.162277660E-3, 1.0, 2.0, 3.162277660, 4.0/ HE SD 018
      HE SD 019
      HE SD 020
      HE SD 021
      HE SD 022
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      HE SD 067
      HE SD 068
      HE SD 069

      C START WITH STEPLENGTH 1.0E-3, REPEATEDLY DIVIDE BY
      C SQRT10. ITERATION STOPS WHEN DIFFERENCE BETWEEN SUCCESSIVE
      C HESIANS LESS THAN 1.0E-6. IF NO SUCCESS IN 5 ITERATIONS,
      C USE RESULT WITH STEPLENGTH 1.0E-4.
      C DIFFERENCE IS MAX. DIFFERENCE BETWEEN SUCCESSIVE ELEMENTS-
      C ABSOLUTE DIFFERENCE IF /LATEST ELEMENT/ LT. 1,
      C RELATIVE DIFFERENCE IF /LATEST ELEMENT/ .GE. 1.
      C
      C ITER = 0
      STEP = STEP1
      DO 10 I = 1, NVAR
      DO 10 J = 1, NVAR
      10 SAVE1(I,J) = ZERO
      C
      C 20 ITER = ITER + 1
      STEP = STEP / SQRT10
      C
      C DIAGONAL ELEMENTS. THREE POINT DIFFERENCING.
      DENOM = STEP * STEP
      DO 30 I = 1, NVAR
      IND = ISUB(I)
      PAR1 = PAR(IND)
      PAR(IND) = PAR1 + STEP
      CALL FUNCT(0, NPAR, PAR, TEMP, PAR, IW, LIW, W, LW)
      PAR(IND) = PAR1 - STEP
      CALL FUNCT(0, NPAR, PAR, TEMP1, PAR, IW, LIW, W, LW)
      TEMP = TEMP + TEMP1
      PAR(IND) = PAR1
      CALL FUNCT(0, NPAR, PAR, TEMP1, PAR, IW, LIW, W, LW)
      H(I,I) = (TEMP - TWO*TEMP1) / DENOM
      30 CONTINUE
      IF (NVAR .EQ. 1) GO TO 50
      C
      C OFF-DIAGONAL ELEMENTS IF REQUIRED. FOUR POINT DIFFERENCING.
      DENOM = FOUR * DENOM
      IND = NVAR - 1
      DO 40 I = 1, IND
      IND1 = I + 1
      IND2 = ISUB(I)
      PAR1 = PAR(IND2)
      DO 40 J = IND1, NVAR
      IND3 = ISUB(J)
      PARJ = PAR(IND3)
      PAR(IND2) = PAR1 + STEP
      PAR(IND3) = PAR1 + STEP
      CALL FUNCT(0, NPAR, PAR, TEMP, PAR, IW, LIW, W, LW)
      PAR(IND3) = PAR1 - STEP
      CALL FUNCT(0, NPAR, PAR, TEMP1, PAR, IW, LIW, W, LW)
      TEMP = TEMP - TEMP1
      PAR(IND2) = PAR1 - STEP

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CALL FUNCT(0, NPAR, PAR, TEMP1, PAR, IW, LIW, W, LW)          HESD 070
TEMP = TEMP + TEMP1                                         HESD 071
PAR(IND3) = PARJ + STEP                                     HESD 072
CALL FUNCT(0, NPAR, PAR, TEMP1, PAR, IW, LIW, W, LW)          HESD 073
H(I,J) = (TEMP - TEMP1) / DENOM                           HESD 074
PAR(IND2) = PARI                                         HESD 075
PAR(IND3) = PARJ                                         HESD 076
40 CONTINUE                                              HESD 077
HESD 078
C   FIND DIFFERENCE, SAVE OLD HESSIAN IN SAVE1.           HESD 079
C   50 TEMP = ZERO                                         HESD 080
DO 60 I = 1, NVAR                                         HESD 081
DO 60 J = 1, NVAR                                         HESD 082
PARI = H(I,J)
TEMP1 = ABS(PARI - SAVE1(I,J))                            HESD 083
PARJ = ABS(PARI)                                         HESD 084
IF (PARJ .GE. ONE) TEMP1 = TEMP1 / PARJ                  HESD 085
TEMP = AMAX1(TEMP, TEMP1)                                HESD 086
SAVE(I,J) = PARI                                         HESD 087
60 CONTINUE                                              HESD 088
HESD 089
C   THIRD ITN, SAVE OLD HESSIAN IN SAVE2 (STEPLNGTH 1.0E-4). HESD 090
IF (ITER .NE. 3) GO TO 80                                 HESD 091
DO 70 I = 1, NVAR                                         HESD 092
DO 70 J = 1, NVAR                                         HESD 093
70 SAVE2(I,J) = H(I,J)                                    HESD 094
HESD 095
C   TEST STOPPING CRITERION FOR ITERATION.                 HESD 096
C   80 IF (TEMP .LT. TOL) GO TO 100                         HESD 097
IF (ITER .LT. 5) GO TO 20                                 HESD 098
HESD 099
C   NO CONVERGENCE IN 5 ITNS - USE SAVE2, WITH STEP TEMP1. HESD 100
STEP = TEMP1
DO 90 I = 1, NVAR                                         HESD 101
DO 90 J = 1, NVAR                                         HESD 102
90 H(I,J) = SAVE2(I,J)                                    HESD 103
HESD 104
C   EXIT, WRITE DETAILS (IND IS OUTPUT UNIT PASSED THROUGH IW), HESD 105
C   AND SAVE THE NUMBER OF ITERATIONS REQUIRED.            HESD 106
C   100 IND = IW(4)                                         HESD 107
IW(1) = ITER                                             HESD 108
IF (IND .GT. 0) WRITE (IND,1000) ITER, STEP               HESD 109
HESD 110
C   1000 FORMAT (16H0HESSIAN DONE IN, 13, 6H ITNS., 16H STEPSIZE USED =, HESD 111
HESD 112
HESD 113
HESD 114
HESD 115
HESD 116
HESD 117
C   RETURN
END

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) This paper presents several families of algorithms for estimation of the parameters of the stable laws and the parameters of attracting stable laws. The paper also presents algorithms for estimation of the parameters of stable regression and stable autoregression models.			

